

Predictive dislocation mobility in high-entropy alloys without driven molecular dynamics: A quantum statistical approach

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We develop a quantum statistical theory of phonon-mediated dislocation drag in chemically disordered alloys. Starting from a configuration-dependent harmonic Hamiltonian with Kanzaki coupling, we integrate out the lattice exactly via a Keldysh influence functional and obtain, for each disordered realization, a causal retarded memory kernel for the collective glide coordinate. The drag coefficient required by continuum mobility laws is the zero-frequency limit of this kernel, rather than an empirical input, while the full kernel provides a principled non-Markovian mobility law. To make the theory tractable for large disordered supercells with *ab initio* methods and machine-learned interatomic potentials, we introduce a hybrid embedding scheme that retains the disorder-sensitive Kanzaki vertex in an inner atomistic region and couples it to an outer effective medium description for far-field phonon radiation. We prove that any procedure which homogenizes the lattice before evaluating the quadratic dissipation functional produces a strict lower bound on the disorder-averaged drag, missing a non-negative variance contribution that is discarded by construction. Calculations for bcc AlW_{0.5}Mo_{0.5}+TiFe, and for face-centered cubic FeCoNi+CuCr systems show that this variance term is typically dominant: virtual crystal estimates underpredict drag by factors of 2 to 8 and suppress the screw versus edge hierarchy predicted by the full theory. The composition dependence is strongly nonmonotonic, demonstrating that chemical complexity alone is not a reliable proxy for drag and that extrapolations based on bulk elastic descriptors or Leibfried-type scaling can fail. Temperature dependence follows analytically from Bose reweighting of a single equilibrium spectral density, recovering the high-temperature linear regime with a slope set by an infrared-weighted spectral moment that remains sensitive to core-level chemistry. The resulting Stieltjes pole parameters provide a complete, passive, non-Markovian mobility input for mesoscale dislocation dynamics in concentrated alloys, with explicit configurational uncertainty quantification and without driven molecular dynamics, thereby providing a complete representation of dislocation mobility in disordered alloys without the need for costly molecular dynamics simulations.

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I. INTRODUCTION

High-entropy alloys (HEAs) represent a paradigm shift in metallurgical design [1,2]. By combining four or more principal elements in near-equimolar proportions, these materials access regions of compositional space that lie far from the dilute limits around which classical alloy theory was constructed. The resulting chemical complexity confers remarkable mechanical properties: exceptional strength retention at elevated temperatures, outstanding resistance to radiation damage, and tuneable ductility across cryogenic to refractory regimes [3–7]. These characteristics have positioned high-entropy alloys as candidates for next-generation structural materials in aerospace, nuclear, and extreme-environment applications [3]. Yet the very disorder that underpins their technological promise also frustrates the theoretical frameworks traditionally employed to understand plastic deformation.

Dislocation mobility is, arguably, the central quantity linking atomic-scale physics to macroscopic plasticity. The velocity at which dislocations traverse a crystal under applied stress determines strain rate sensitivity, work hardening, creep resistance, and dynamic failure [8,9]. In pure metals, dislocation motion is governed by well-characterized drag mechanisms: at low temperatures, the Peierls barrier dominates in body-centered cubic structures [10], while at higher temperatures, phonon drag becomes rate-limiting [9]. The drag coefficient B entering the mobility law $v = \tau b/B$ encapsulates the dissipative coupling between the moving dislocation and the host lattice [8]. Despite decades of theoretical effort, even in pure crystals, the microscopic origin of this coefficient remains incompletely understood, with discrepancies persisting between lattice theoretical [11–13], continuum elastodynamic predictions [14,15], atomistic simulations [16–18], and experimental measurements [19,20].

The situation in high-entropy alloys is considerably more opaque. Chemical disorder on an otherwise crystalline lattice breaks translational invariance, introduces local lattice distortions [21–23], broadens vibrational spectra [24,25], and creates spatial fluctuations in elastic moduli that vary on length scales comparable to the dislocation core [26,27]. These features invalidate the Bloch symmetry that underpins

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phonon drag theories in ordered crystals and render the dilute-limit perturbation expansions of classical solid solution strengthening inapplicable. A framework that remains well-defined without translational invariance is therefore required if one aims to connect atomistic modeling to a macroscopic drag coefficient suitable for dislocation dynamics in concentrated alloys.

Existing approaches to dislocation behavior in high-entropy alloys fall into several methodological categories, each with characteristic strengths and limitations. Molecular dynamics simulations, particularly those employing machine-learned interatomic potentials [28], have provided invaluable mechanistic insight. Studies using moment tensor potentials [29] on refractory systems such as MoNbTaW have revealed that edge-to-screw mobility ratios differ dramatically from pure body-centered cubic metals [30], that jerky glide originates from local Peierls friction fluctuations [31,32], or that chemical short-range order affects edge and screw dislocations through opposite mechanisms [32–34]. These simulations have extracted drag coefficients directly from velocity-stress relations [30,35,36] and have identified phenomena invisible to continuum theories, including cross-kink pinning [37] and line-length-dependent mobility [35]. However, molecular dynamics is fundamentally classical: it captures phonon-mediated dissipation through empirical or fitted potentials but cannot access electronic contributions to drag. Furthermore, their computational cost is high, as each point in a nominal velocity-stress mobility relation requires costly and lengthy simulations, to which, in the case of HEAs, one must add the need to repeat said data point over an ensemble of different lattice arrangements to capture ensemble statistics correctly [6,34]. Moreover, the strain rates accessible to simulation exceed experimental values by eight to twelve orders of magnitude, and the dislocation segments modeled are orders of magnitude shorter than those observed experimentally.

First-principles calculations based on density functional theory (DFT) have addressed complementary aspects of the problem. *Ab initio* studies have characterized screw dislocation core structures in refractory high-entropy alloys [38], mapped Peierls energy landscapes across compositional space [39–41], and quantified the distribution of core energies arising from chemical fluctuations [42]. These calculations provide essential input (i.e., elastic constants, stacking fault energies, Peierls barriers) but do not directly yield mobility or drag coefficients, which must be fitted to higher-order mobility theories instead. The computational expense of density functional theory restricts such studies to static configurations or to nudged elastic band calculations of migration barriers [43], leaving the dynamical coupling between dislocation motion and lattice excitations unaddressed.

A common thread runs through these atomistic approaches: each molecular dynamics trajectory or density functional calculation represents a single disordered realization, and extracting macroscopically meaningful quantities requires averaging over a potentially large ensemble of configurations. This averaging compounds an already substantial computational cost, particularly for properties like dislocation mobility that demand large simulation cells, long equilibration times, and systematic sampling of stress and temperature. It is for

this reason that a substantial body of work on disordered alloys relies on effective medium descriptions, which replace the disordered lattice with a translationally invariant surrogate that captures certain averaged properties of the crystal. The simplest such description is the virtual crystal approximation (VCA), which substitutes each lattice site with a fictitious atom having composition-weighted mass, pseudopotential, and force constants [44]. More sophisticated is the coherent-potential approximation (CPA), introduced by Soven [45] and married to the Korringa–Kohn–Rostoker (KKR) [46,47] multiple scattering formalism by Györfy [48], which determines the effective medium self-consistently by requiring that the average scattering from the true atomic species embedded in the effective medium vanishes. The KKR-CPA and its descendants [including the EMTO-CPA code [49] and the surface-plasmon resonance (SPR) KKR implementation [50]] have become standard tools for computing electronic structure, elastic constants, and magnetic properties of disordered alloys across vast compositional spaces [51,52].

For lattice dynamics, effective medium approaches face additional challenges. The VCA produces spurious band gaps in phonon dispersions when constituent masses differ substantially [24], while standard CPA treats only mass disorder and neglects force-constant fluctuations. The itinerant CPA theory [53] addresses this by incorporating force-constant disorder self-consistently, and has been applied to phonon scattering in binary alloys and, more recently, to high-entropy systems [24,54]. These calculations reveal that both mass and force constant fluctuations contribute comparably to phonon linewidths, and that neglecting either produces qualitatively incorrect results. Cluster extensions of these ideas, including dynamical cluster approaches and typical medium formulations, go beyond single-site averaging by retaining nonlocal disorder correlations and by distinguishing arithmetic from typical spectral response in the presence of strong disorder [55–58]. These developments are important for bulk disordered phonons, especially when spectral broadening and localization are substantial.

A complementary approach avoids effective media altogether by constructing explicit supercells that mimic the statistics of random disorder. Special quasirandom structures (SQSs) [59] are small periodic cells whose short-range correlation functions match those of a random alloy. SQS calculations capture local lattice distortions that effective medium theories cannot represent [60,61], and systematic comparisons show that CPA and SQS predictions diverge precisely when relaxation effects dominate [62]. However, SQS calculations scale poorly with system size and provide only a single disorder realization, limiting their utility for properties that depend on configurational fluctuations alone.

It is for this reason that, for mechanical properties, the dominant theoretical framework is the Varvenne–Curtin–Leyson theory [63,64] and its extensions [39,65], which rests explicitly on effective medium foundations inherited from Labusch’s statistical theory of solid solution strengthening [66]. This approach treats the random alloy as an effective homogeneous medium in which each elemental component acts as a fluctuation about the averaged matrix. Strengthening arises from dislocation interactions with these fluctuations, yielding parameter-free predictions of zero-temperature yield

stress from misfit volume data. The theory has been validated against experiments on face-centered cubic (fcc) systems from cryogenic to elevated temperatures [67,68], and extensions to body-centered cubic (bcc) refractory alloys [65,69,70] identified distinct strengthening regimes controlled by kink-pair nucleation, lateral kink glide, and cross-kink failure.

These models provide valuable predictive estimates of strength, yet they share with all effective medium approaches a mathematical limitation that has not been widely appreciated. As we discuss in this work, the quantities controlling radiated power and phonon drag are not linear in disorder but involve quadratic forms in configuration-dependent couplings and propagators. Replacing the disordered lattice with an averaged effective medium before evaluating these quadratic forms systematically underestimates the result, because the average of a quadratic functional is not the quadratic functional of the averages. The discrepancy is precisely the variance contribution induced by chemical disorder, a contribution that effective medium theories discard by construction. This limitation applies equally to VCA, CPA, and the mechanical theories built upon any such effective medium: any observable that depends quadratically on local atomic environments will be underestimated when those environments are replaced by their mean.

This observation motivates the present work. We develop a quantum statistical framework for dislocation drag in disordered crystals that is exact within the harmonic approximation and that correctly handles configurational averaging. Recently introduced for conventional ordered systems [71], the formalism combines two ingredients: a Kanzaki source representation of Volterra slip, which encodes the dislocation as a classical source acting on the lattice, and a Keldysh influence functional for the harmonic phonon bath, which integrates out lattice degrees of freedom to yield a closed dynamical equation for the collective glide coordinate. For each disordered configuration, the construction produces a configuration-resolved retarded memory kernel with the Stieltjes structure characteristic of oscillator baths. The high-entropy alloy kernel is then obtained by averaging the spectral density, not the harmonic operator, over disordered realizations. This quenched averaging preserves the variance contribution that effective medium theories lose and yields memory kernels that correctly account for disorder-enhanced drag.

To render the formalism computationally viable with machine-learned interatomic potentials (i.e., Ref. [72]), we introduce a controlled hybrid embedding. An inner atomistic region containing the dislocation core determines the configuration-dependent Kanzaki source and retains full chemical disorder. An outer effective infinite medium supplies the correct radiation condition and long-range propagation at low cost. The embedding self-energy couples the two regions without introducing spurious reflections at the interface. This separation confines the expensive disorder-sensitive physics to a small region, while the far-field propagation that enforces the effective one-dimensional character of the drag is handled by a cheap translationally invariant operator. After configurational averaging, the resulting high-entropy alloy kernels recover the same Stieltjes hierarchy as in ordered crystals, with the ordered spectral densities replaced by their disorder-averaged counterparts. We provide adequate bounds

and coherence ratios to ensure that the embedding strategy remains a faithful representation of the disordered lattice.

The framework developed here is not a refinement of existing approaches, but rather a conceptual reorientation. Rather than extracting mobility phenomenologically from simulation trajectories or estimating strength from static energy barriers, we derive dislocation dynamics from the quantum statistical mechanics of a coupled system-dislocation interaction with a disordered thermal bath. The retarded kernel encapsulates all linear-response information about phonon-mediated drag, including memory effects that are invisible to instantaneous friction models and extremely difficult to measure in molecular dynamics (MD) simulations. The spectral density provides a unified language for comparing different alloy compositions, identifying frequency regimes that dominate dissipation, and ultimately extending the formalism to include electronic drag through analogous influence functional constructions. By grounding the theory in causal response functions and proper ensemble averaging, the approach bridges atomistic detail and continuum-scale dislocation dynamics without sacrificing analytical tractability.

The remainder of this article is organized as follows. Section II establishes the Keldysh–Kanzaki formalism for a disordered alloy. We define the configuration-dependent harmonic Hamiltonian, introduce the Kanzaki representation of a straight dislocation, and derive the configuration-resolved effective action and memory kernels. Section III demonstrates why replacing disorder by an effective medium is not equivalent to averaging over disorder realizations, identifying the variance contribution that effective medium theories omit. Section IV develops the hybrid embedding scheme that separates an atomistic inner region from an effective medium outer region, describes the embedding self-energy, and shows how the construction preserves the Stieltjes structure of the memory kernel. Section V formulates the matrix-valued spectral measures and retarded kernels for a dislocation dipole, derives the projection that recovers the single-line drag from the dipole observable, and establishes the coherence ratio diagnostic that controls the accuracy of this extraction. Section VI outlines the computational pipeline from machine-learned interatomic potential evaluations to configurationally averaged drag coefficients. Section VII presents results for dislocation drag in medium- and high-entropy alloys, comparing configuration-resolved and averaged kernels, demonstrating the enhancement of drag by chemical variance, and extracting non-Markovian mobility laws from the Stieltjes pole structure. Section VIII summarizes the principal conclusions and identifies directions for future development, including extension to electronic drag, anharmonicities, and collective dislocation phenomena.

II. KELDYSH–KANZAKI FORMALISM FOR DISLOCATION MOBILITY IN DISORDERED ALLOYS

We construct a microscopic description of phonon-mediated dissipation for a straight dislocation in a chemically disordered alloy. For each fixed disorder realization C , we integrate out the harmonic lattice fluctuations coupled to the dislocation through a Kanzaki source, which yields a configuration-resolved influence action for the glide

coordinate $X(t)$. The influence action is fully characterized by two kernels: a retarded kernel, which encodes the causal backaction of the lattice and hence the mobility memory kernel, and a Keldysh kernel, which fixes the symmetrized force fluctuations through the fluctuation dissipation relation. The low velocity drag coefficient and the steady radiated power are not introduced phenomenologically, but arise as the uniform glide limit and the zero-frequency limit of the retarded kernel. We then define the high-entropy alloy kernel by configurational averaging at the level of the kernels themselves; this ordering is essential because the influence functional is linear in the configuration ensemble, whereas any finite pole representation is a nonlinear postprocessing step.

Throughout this section, the lattice degrees of freedom are assumed to be in thermal equilibrium at a fixed temperature T , described by a canonical density matrix for the harmonic phonon Hamiltonian of each disorder configuration. The dislocation coordinate is treated as a slow collective variable coupled linearly to this thermal phonon bath through the Kanzaki force. The main text gives the configuration-resolved Hamiltonian, the Kanzaki interaction, the normal-mode coupling, the influence action, and the spectral objects entering the mobility law. Details of the discrete Volterra construction, the expansion of the shifted harmonic Hamiltonian, the mode normalization, and the explicit contour integration are collected in Appendix A.

A. Configuration-resolved Hamiltonian, Kanzaki coupling, and influence action

We consider a substitutionally disordered solid solution on a Bravais lattice with sites $\mathbf{R}$ and chemical variables $\{\sigma_{\mathbf{R}}\}$. A particular alloy realization is denoted $C \equiv \{\sigma_{\mathbf{R}}\}$. For that fixed C we define a three-component displacement field $u_i(\mathbf{R}, t)$ and conjugate momenta $p_i(\mathbf{R}, t)$. The harmonic phonon Hamiltonian is

$$H_{\text{ph}}^{(C)} = \frac{1}{2} \sum_{\mathbf{R}} \frac{p_i(\mathbf{R}) p_i(\mathbf{R})}{M_C(\mathbf{R})} + \frac{1}{2} \sum_{\mathbf{R}, \mathbf{R}'} u_i(\mathbf{R}) \Phi_{ij}^{(C)}(\mathbf{R}, \mathbf{R}') u_j(\mathbf{R}'), \quad (1)$$

where the local masses $M_C(\mathbf{R})$ and the force constant matrix $\Phi_{ij}^{(C)}(\mathbf{R}, \mathbf{R}')$ depend on the chemical configuration C . In the absence of sources, the static Euler equation reads

$$\sum_{\mathbf{R}'} \Phi_{ij}^{(C)}(\mathbf{R}, \mathbf{R}') u_j(\mathbf{R}'; C) = 0. \quad (2)$$

We now introduce a straight dislocation with Burgers vector $\mathbf{B}$ and line direction $\hat{\mathbf{z}}$, gliding in the x direction, as shown in Fig. 1. The discrete Volterra construction fixes the Burgers topology and the displacement discontinuity across the slip surface; the corresponding bond indicator, jump condition, and slip form factor are given in Appendix A 1. In the main text, we use the equivalent Kanzaki representation. We denote by $u^V(\mathbf{R}; X)$ a Volterra representative carrying the far-field elastic structure, and by $u^{\text{slip}}(\mathbf{R}; X; C)$ the complete static displacement obtained after core relaxation and local distortion in configuration C . The Kanzaki force [73,74] is defined as the source that reproduces u^{slip} within the harmonic lattice

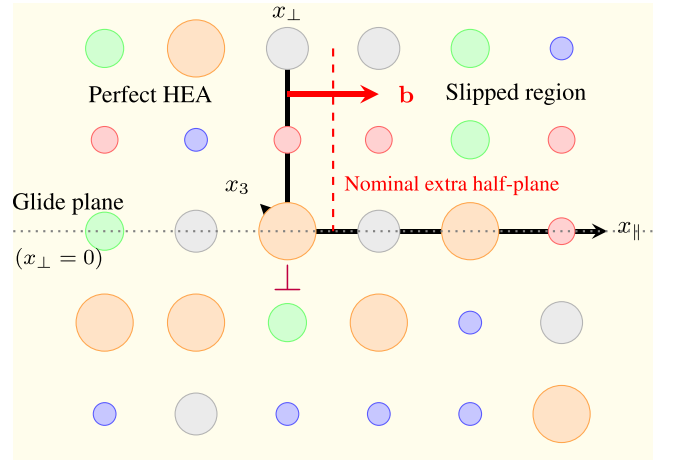


FIG. 1. Two-dimensional view of an edge dislocation in the glide plane. The coordinate system has $x_{\parallel}$ as the glide direction, $x_{\perp}$ normal to the glide plane, and x_3 along the dislocation line (perpendicular to the page). The dislocation core is marked by $\perp$, with the extra half plane of atoms (dashed red line) terminating at the core. The Burgers vector $\mathbf{b}$ and glide velocity v_d are both parallel to $x_{\parallel}$. For a screw dislocation, the Burgers vector would be parallel to x_3 .

operator $\Phi^{(C)}$,

$$f_i^K(\mathbf{R}; X; C) \equiv \sum_{\mathbf{R}'} \Phi_{ij}^{(C)}(\mathbf{R}, \mathbf{R}') u_j^{\text{slip}}(\mathbf{R}'; X; C). \quad (3)$$

In practice, one may impose the Volterra displacement u^V as a boundary condition, compute the resulting harmonic forces $\sum_{\mathbf{R}'} \Phi^{(C)}(\mathbf{R}, \mathbf{R}') u^V(\mathbf{R}')$, and identify the nonzero forces near the core as the Kanzaki field f^K [75,76]. Once Eq. (3) holds, the dislocation can be treated as a classical source acting on the otherwise harmonic lattice.

The total displacement is split into a deterministic slip field and a fluctuation field,

$$u_i(\mathbf{R}, t) = u_i^{\text{slip}}(\mathbf{R}; X(t); C) + u_i^{\text{ph}}(\mathbf{R}, t; C). \quad (4)$$

The expansion of Eq. (1) under this shift is given in Appendix A 1. It produces a static elastic contribution, absorbed into the dislocation Hamiltonian, and a term linear in u^{ph} . With the usual source convention in the action, this gives the interaction Hamiltonian

$$H_{\text{int}}^{(C)}[X, u^{\text{ph}}] = - \sum_{\mathbf{R}, i} f_i^K(\mathbf{R}; X; C) u_i^{\text{ph}}(\mathbf{R}; C), \quad (5)$$

and the full Hamiltonian for configuration C becomes

$$H^{(C)} = H_{\text{ph}}^{(C)}[u^{\text{ph}}, p] + H_{\text{dis}}[X, P_X; C] + H_{\text{int}}^{(C)}[X, u^{\text{ph}}]. \quad (6)$$

In this representation, the static elastic field generated by the dislocation is contained in $H_{\text{dis}}[X, P_X; C]$, while the thermal and quantum lattice fluctuations enter through a linear Kanzaki coupling.

For each configuration C , let $\omega_{\nu C}$ and $e_i^{(\nu C)}(\mathbf{R})$ denote the phonon frequencies and physical eigenvectors of the mass-weighted harmonic operator, with the mode normalization and displacement expansion stated in Appendix A 2. The har-

monic Hamiltonian diagonalizes as

$$H_{\text{ph}}^{(C)} = \sum_v \hbar \omega_{vC} \left(a_{vC}^\dagger a_{vC} + \frac{1}{2} \right). \quad (7)$$

Substitution of the mode expansion into Eq. (5) gives

$$H_{\text{int}}^{(C)}[X] = - \sum_v g_{vC}(X) (a_{vC} + a_{vC}^\dagger), \quad (8)$$

with configuration-dependent Kanzaki mode couplings

$$g_{vC}(X) = \sqrt{\frac{\hbar}{2M_{\text{ref}}\omega_{vC}}} \sum_{\mathbf{R},i} f_i^K(\mathbf{R}; X; C) e_i^{(vC)}(\mathbf{R}). \quad (9)$$

The quantities in Eqs. (7) and (8) are the only lattice ingredients required for the Keldysh construction: a Gaussian bath and a linear source coupling.

When modeling dislocation mobility, a purely Hamiltonian treatment is insufficient because phonon-mediated drag is dissipative and accompanied by thermal force fluctuations. The Keldysh contour formulation [77–80] provides the framework in which the causal lattice response and the symmetrized force correlations are obtained from the same microscopic coupling. The closed time contour functional and the Gaussian integration over $u_\pm^{\text{ph}}$ are given in Appendix A3; here we quote the resulting influence action.

Introducing classical and quantum combinations [79,80]

$$X_c(t) = \frac{X_+(t) + X_-(t)}{\sqrt{2}}, \quad X_q(t) = \frac{X_+(t) - X_-(t)}{\sqrt{2}}, \quad (10)$$

and expanding the influence action to second order in X_q , one obtains

$$S_{\text{eff}}^{(C)}[X_c, X_q] = S_{\text{dis}}[X_c, X_q] - \frac{1}{2} \int dt dt' X_q(t) \mathcal{D}_C^R(t-t') X_c(t') - \frac{i}{2} \int dt dt' X_q(t) \mathcal{N}_C(t-t') X_q(t'), \quad (11)$$

where $\mathcal{D}_C^R(t)$ is the configuration dependent retarded kernel and $\mathcal{N}_C(t)$ is the corresponding Keldysh noise kernel. Formally, this is the disordered analog of the ordered construction, obtained through the substitutions

$$\mathcal{D}^R(t) \rightarrow \mathcal{D}_C^R(t), \quad \mathcal{N}(t) \rightarrow \mathcal{N}_C(t), \quad (12)$$

with all phonon data carrying the configuration label C . The retarded kernel governs the deterministic backaction of the lattice, while the Keldysh kernel fixes the symmetrized force fluctuations. For a harmonic bath in thermal equilibrium, these kernels obey the fluctuation-dissipation relation.

Varying Eq. (11) with respect to X_q and then setting $X_q = 0$ gives the configuration-resolved stochastic equation of motion

$$\frac{\delta S_{\text{dis}}}{\delta X_c(t)} - \int dt' \mathcal{D}_C^R(t-t') X_c(t') = \xi_C(t), \quad (13)$$

where $\xi_C(t)$ is the stochastic force with correlator fixed by $\mathcal{N}_C(t)$. For the mobility problem, the retarded term is rewritten as a causal functional of the glide velocity by expanding the Kanzaki source about a reference trajectory, following the ordered construction of Ref. [71]. The deterministic force is decomposed as

$$F_{\text{det}}^{(C)}[X](t) = F_{\text{cons}}^{(C)}[X](t) + F_{\text{drag}}^{(C)}[X](t), \quad (14)$$

where $F_{\text{cons}}^{(C)}$ collects the conservative Peach–Koehler and Peierls forces. In the linear mobility regime,

$$F_{\text{drag}}^{(C)}[X](t) = - \int_0^\infty \Gamma_{T,C}(\tau) \dot{X}(t-\tau) d\tau + O(\dot{X}^3), \quad (15)$$

where $\Gamma_{T,C}(t) \equiv \Gamma_{T,C}^{(1)}(t)$ is the configuration-resolved linear mobility kernel obtained from $\mathcal{D}_C^R$ after line projection. For uniform glide, causality gives

$$F_{\text{drag}}^{(C)}(v_d) = -v_d \int_0^\infty \Gamma_{T,C}(\tau) d\tau = -v_d \hat{\Gamma}_{T,C}(0) \equiv -B_{T,C} v_d, \quad (16)$$

so that the conventional viscous drag law follows as the zero-frequency limit of the retarded mobility kernel, with no phenomenological input.

B. Radiated power and line-projected spectral densities for a single configuration

For a fixed disorder configuration C , the instantaneous mechanical power transferred from the dislocation to the lattice is

$$P^{(C)}(t) = \dot{X}(t) F_{\text{drag}}^{(C)}[X](t), \quad (17)$$

where only the drag part of the force contributes to dissipation. In the stationary state corresponding to uniform glide at a constant velocity v_d ,

$$X(t) = v_d t, \quad \dot{X}(t) = v_d. \quad (18)$$

Equation (16) gives the configuration-resolved linear drag force. The time-averaged radiated power is then

$$P^{(C)}(v_d) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \dot{X}(t) F_{\text{drag}}^{(C)}(v_d) = v_d F_{\text{drag}}^{(C)}(v_d), \quad (19)$$

so that, to leading order in v_d ,

$$P^{(C)}(v_d) = v_d^2 \hat{\Gamma}_{T,C}^{(1)}(0). \quad (20)$$

At zero temperature, this expression represents dissipation arising solely from quantum zero-point fluctuations of the lattice. At finite temperature, the same expression acquires an additional contribution from thermally populated phonon modes through the Bose occupation factors entering the spectral density, leading to the familiar enhancement of drag with temperature. A fully detailed account of this thermal dependency is given in Appendix C, where we show that at high temperature the drag coefficient is $\propto T$, and in the low-temperature limit, is $\propto T^5$, in agreement with semiphenomenological accounts of phonon drag [8,13,81].

Equation (20) is the exact configuration-resolved analog of the ordered result: the same line-projected kernel $\Gamma_{T,C}^{(1)}$ which governs the nonlocal friction also determines the energy radiated into phonons at constant velocity. It motivates the introduction of the configuration-specific drag coefficient

$$B_{T,C}^{(1)} \equiv \hat{\Gamma}_{T,C}^{(1)}(0), \quad (21)$$

so that $P^{(C)}(v_d) = B_{T,C}^{(1)} v_d^2$ at low velocities. In the following, we express $\hat{\Gamma}_{T,C}^{(n)}(s)$ in terms of the configuration-resolved

spectral densities constructed from the Kanzaki mode couplings, and then perform the configurational average appropriate to the high-entropy alloy.

To make contact with the microscopic phonon modes, we now project the force $F_X^{(C)}$ onto the dislocation line direction. For each configuration C , we introduce an effective line wave number $k_{\parallel, \nu C}$ and a longitudinal slip-phonon vertex $C_{\nu C}$ for mode ν , defined by projecting the Kanzaki force gradient onto the phonon eigenvector and the glide direction,

$$C_{\nu C} = -\sqrt{\frac{\hbar}{2M_{\text{ref}}\omega_{\nu C}}} \sum_{\mathbf{R}, i} [\partial_X f_i^K(\mathbf{R}; X; C)] e_i^{(\nu C)}(\mathbf{R}), \quad (22)$$

and defining the line parallel wave-number content of the mode by its plane-wave weight along the dislocation line. Writing the line coordinate as x and restricting to atoms within a fixed transverse window around the line, we introduce the normalized weight $w_{\nu C}(k_{\parallel}) \geq 0$ obtained from the squared modulus of the discrete Fourier transform of $e^{(\nu C)}$ along x . In the ordered crystal $w_{\nu C}$ collapses to a delta peak at the Bloch wave number $k_{\parallel}$, whereas in a disordered alloy it is generally broadened or multimodal. Since the Doppler reduction couples to moments of the line wave number, we therefore replace the single number $k_{\parallel, \nu C}$ by the moment functional $\kappa_{\nu C}^{(n)} \equiv \int dk_{\parallel} w_{\nu C}(k_{\parallel}) |k_{\parallel}|^{2n-1}$, which reduces to $|k_{\parallel}|^{2n-1}$ in the Bloch limit and remains well-defined for fragmented or partially localized modes.

With these definitions, the configuration-resolved line-projected spectral densities are obtained by direct analogy with the ordered case, replacing the ordered mode data $\{\omega_{\lambda}, C_{\lambda}, k_{\parallel, \lambda}\}$ by $\{\omega_{\nu C}, C_{\nu C}, k_{\parallel, \nu C}\}$:

$$\rho_n^C(\Omega) = \frac{\hbar}{\varrho} \sum_{\nu} \frac{\kappa_{\nu C}^{(n)}}{n!} \frac{|C_{\nu C}|^2}{\omega_{\nu C}} \delta(\Omega - \omega_{\nu C}), \quad n = 0, 1, 2, \dots, \quad (23)$$

where ϱ is the mass density [reserved to avoid notational collision with the spectral density $\rho_n^C(\Omega)$] and $n_B(\omega) = (e^{\beta\hbar\omega} - 1)^{-1}$. Note that the line-projected spectral density $\rho_n^C(\Omega)$ defined above characterizes the strength with which a moving dislocation couples to lattice vibrations of frequency Ω in configuration C . It is a purely mechanical object, determined entirely by the harmonic force constants and Kanzaki vertices, and is independent of temperature. All thermal effects enter subsequently through the equilibrium occupation of these modes.

The case $n = 1$ governs the linear drag and appears in Eq. (20); as stated above, higher n encode nonlinear corrections in the slip velocity. In the ordered limit, the sum over ν becomes a sum over branches and Brillouin-zone wave vectors, and Eq. (23) reduces to the Brillouin-zone expressions used previously.

Thermal effects appear when constructing physical observables from the spectral density. In particular, the symmetrized force correlations involve the thermal phonon occupation factors and are therefore weighted by the equilibrium Bose function, as dictated by the fluctuation-dissipation relation for a harmonic bath. For later use, we thus define the thermal (Keldysh) spectral density $\rho_n^{C, K}(\Omega) \equiv [2n_B(\Omega) + 1] \rho_n^C(\Omega)$, which controls the symmetrized force fluctuations. The drag

and radiated power are governed by the retarded kernel constructed from ρ_n^C , while $\rho_n^{C, K}$ enters the noise correlator through the fluctuation dissipation relation.

C. Line-projected memory kernels in Laplace space

The influence functional derived above generates a hierarchy of line-projected memory kernels $\Gamma_{T, C}^{(n)}(t)$ multiplying odd powers of the slip velocity, corresponding to successive terms in the expansion of the retarded force functional about $\dot{X} = 0$. The index n labels the order in this expansion and has a clear physical interpretation: $n = 1$ governs the linear mobility regime and determines the drag coefficient, while $n \geq 2$ encode nonlinear corrections relevant only at higher velocities. In the remainder of this work, we retain explicitly only the $n = 1$ kernel, which is sufficient for the low velocity regime of interest, and we keep the index n here solely to make contact with the general structure of the theory.

For a fixed disorder configuration C , the Laplace transform of the n th-order kernel can be written directly in terms of the corresponding line-projected spectral density defined in Eq. (23) as

$$\hat{\Gamma}_{T, C}^{(n)}(s) = s \int_0^\infty d\Omega \frac{\rho_n^C(\Omega)}{s^2 + \Omega^2}, \quad \text{Re } s > 0. \quad (24)$$

This representation is exact within the harmonic approximation and shows that all non-Markovian memory effects are fully encoded in the mechanical spectral density $\rho_n^C(\Omega)$. Importantly, $\rho_n^C(\Omega)$ is independent of temperature; the temperature dependence of physical observables enters only through equilibrium occupation factors when constructing noise correlators or finite-temperature averages, as dictated by the fluctuation-dissipation relation [71, 79, 82].

The quantities relevant for practical mobility laws are obtained from the low-frequency expansion of $\hat{\Gamma}_{T, C}^{(n)}(s)$ [71]:

$$\hat{\Gamma}_{T, C}^{(n)}(s) = \int_0^\infty d\Omega \frac{\rho_n^C(\Omega)}{\Omega + s}, \quad (25)$$

so that, for $|s|$ small compared with the spectral support, one has the convergent expansion

$$\begin{aligned} \hat{\Gamma}_{T, C}^{(n)}(s) &= \int_0^\infty d\Omega \frac{\rho_n^C(\Omega)}{\Omega} - s \int_0^\infty d\Omega \frac{\rho_n^C(\Omega)}{\Omega^2} \\ &\quad + s^2 \int_0^\infty d\Omega \frac{\rho_n^C(\Omega)}{\Omega^3} + \dots, \end{aligned} \quad (26)$$

where the coefficients are inverse moments of the projected spectral density.

The leading term defines the configuration-resolved moment

$$B_{T, C}^{(n)} \equiv \hat{\Gamma}_{T, C}^{(n)}(0) = \int_0^\infty d\Omega \frac{\rho_n^C(\Omega)}{\Omega}, \quad (27)$$

which for $n = 1$ coincides with the static drag coefficient entering the linear mobility law. Higher derivatives at $s = 0$ define additional moments,

$$B_{1, C}^{(n)} = \left. \frac{\partial \hat{\Gamma}_{T, C}^{(n)}(s)}{\partial s} \right|_{s=0}, \quad (28)$$

and so on, which quantify the characteristic relaxation times of the kernel and control its frequency dependence.

Inserting Eq. (27) into the uniform glide expression for the radiated power recovers the familiar quadratic dependence at low velocity,

$$P^{(C)}(v_d) \simeq B_{T,C}^{(1)} v_d^2, \quad (29)$$

with higher-order corrections governed by $B_{T,C}^{(n)}$ for $n \geq 2$. Thus, the same spectral density $\rho_n^C(\Omega)$ simultaneously controls the dissipated power and the nonlocal friction kernel for each disorder realization.

In practice, reducing the full kernel $\hat{\Gamma}_{T,C}^{(1)}(s)$ to its zero-frequency value yields a purely viscous mobility law. Retaining additional moments or approximating $\hat{\Gamma}_{T,C}^{(1)}(s)$ by a low-order rational function allows one to construct controlled non-Markovian extensions. The hierarchy of moments introduced here therefore provides the natural bridge between the microscopic spectral representation and the effective mobility laws used in mesoscale modeling.

D. Configuration averaging and HEA kernels

A high-entropy alloy is represented by an ensemble of substitutional disorder configurations C drawn from the appropriate statistical distribution, for instance, a special quasi-random structure ensemble. For each configuration, the Keldysh–Kanzaki construction yields a well-defined hierarchy of line-projected memory kernels $\Gamma_{T,C}^{(n)}(t)$ and corresponding spectral densities $\rho_n^C(\Omega)$, labeled by the order n of the velocity expansion.

The ensemble need not be an uncorrelated random-alloy ensemble. The same construction applies to alloys with short-range order, special quasirandom structures, Monte Carlo or cluster expansion samples, ordered crystals, and experimentally constrained chemical configurations. Short-range order simply changes the probability measure $P(C)$ over quenched configurations; since the force constants, Kanzaki source, Green's function, and projected spectral density are all constructed before averaging, local chemical correlations enter the mobility kernel directly, and no modification of the formalism is required.

The physically meaningful coarse-grained mobility law for the alloy must be constructed by configurational averaging. Crucially, this averaging must be performed at the level of the kernels or, equivalently, at the level of the spectral densities themselves. Averaging fitted parameters, moments, or pole representations obtained from individual configurations is not justified, as the mapping from $\rho_n^C(\Omega)$ to such reduced representations is nonlinear.

Accordingly, we define the disorder-averaged line-projected spectral densities as

$$\rho_n^{\text{HEA}}(\Omega) = \langle \rho_n^C(\Omega) \rangle_C, \quad (30)$$

where $\langle \cdot \rangle_C$ denotes the ensemble average over configurations. Since $\rho_n^C(\Omega)$ is a purely mechanical object determined entirely by the harmonic force constants and Kanzaki vertices, this averaging step isolates the effects of chemical disorder without introducing any thermal assumptions.

Using the linearity of the Stieltjes representation [83], the averaged spectral density immediately defines the disorder-

averaged memory kernel,

$$\hat{\Gamma}_{T,\text{HEA}}^{(n)}(s) = s \int_0^\infty d\Omega \frac{\rho_n^{\text{HEA}}(\Omega)}{s^2 + \Omega^2}, \quad \text{Re } s > 0, \quad (31)$$

which is the exact analog of the configuration-resolved expression in Eq. (24). The corresponding HEA moments are then obtained from the small- s expansion (q.v. Ref. [71]),

$$B_{T,\text{HEA}}^{(n)} = \hat{\Gamma}_{T,\text{HEA}}^{(n)}(0) = \int_0^\infty d\Omega \frac{\rho_n^{\text{HEA}}(\Omega)}{\Omega}, \quad (32)$$

$$B_{1,\text{HEA}}^{(n)} = \left. \frac{\partial \hat{\Gamma}_{T,\text{HEA}}^{(n)}(s)}{\partial s} \right|_{s=0}, \quad (33)$$

and higher derivatives if required.

In the present work, we focus on the linear mobility regime and therefore restrict attention to the $n = 1$ kernel. From this point onward, unless explicitly stated otherwise, we adopt the shorthand $\Gamma_{T,\text{HEA}} \equiv \Gamma_{T,\text{HEA}}^{(1)}$, $\rho^{\text{HEA}}(\Omega) \equiv \rho_1^{\text{HEA}}(\Omega)$, $B_{T,\text{HEA}} \equiv B_{T,\text{HEA}}^{(1)}$. Higher-order kernels $n \geq 2$, which control nonlinear velocity corrections, are not retained in the quantitative analysis reported below, and will be the subject of future work.

Thermal effects enter only after configurational averaging, through the equilibrium occupation of phonon modes. The disorder-averaged retarded kernel $\hat{\Gamma}_{T,\text{HEA}}^{(n)}$ is constructed from $\rho_n^{\text{HEA}}(\Omega)$ alone, while the corresponding noise kernel is fixed by the fluctuation-dissipation relation [79,80] and involves the thermal spectral density

$$\rho_n^{\text{HEA},K}(\Omega) = [2n_B(\Omega) + 1] \rho_n^{\text{HEA}}(\Omega).$$

This separation ensures that chemical disorder and temperature play conceptually distinct roles: disorder reshapes the spectral density, while temperature controls the occupation of those modes. For further details, see Appendix C.

In the absence of chemical disorder, $\rho_n^{\text{HEA}}(\Omega)$ reduces to the ordered spectral density and Eqs. (31)–(33) collapse exactly to the ordered Keldysh–Kanzaki expressions obtained in Ref. [71].

In the following section, the disorder-averaged kernel $\hat{\Gamma}_{T,\text{HEA}}(s)$ obtained here is approximated by a finite n -pole Stieltjes representation. This step provides a compact parametrization of the memory kernel in terms of a small number of relaxation frequencies and weights, which can be embedded directly into mesoscale dislocation dynamics simulations. Importantly, the pole fitting is performed only after configurational averaging of the kernel, ensuring that the resulting parameters represent true ensemble-averaged dissipation channels rather than artifacts of individual disorder realizations.

E. From exact Doppler reduction to disorder-averaged line projections

In an ordered crystal, the reduction of the radiated power and of the mobility kernels to a one-dimensional Doppler integral is exact. It follows from two exact symmetries: translational invariance along the dislocation line and the planar geometry of the Volterra cut. Together, they imply that the Fourier transform of the slip indicator has distributional support only on wave vectors of the form $\mathbf{k} = k_{\parallel} \hat{\mathbf{x}}$, so that the Brillouin-zone integral collapses to a single integral over

$k_{\parallel}$, constrained further by the Doppler resonance condition $\omega_{\alpha}(\mathbf{k}) = v_d k_{\parallel}$. This collapse is thus a direct consequence of symmetry and geometry in the ordered lattice.

Chemical disorder breaks this structure at the level of individual configurations. For a fixed configuration C , translational invariance along the line is lost, Bloch wave vectors are no longer good quantum numbers, and the slip form factor no longer produces exact delta function support in reciprocal space. As a result, the exact configuration-resolved expressions for the radiated power and for the kernels $\Gamma_{T,C}^{(n)}$ involve sums or integrals over the full supercell Brillouin zone, with vertices and mode weights that depend on all components of the wave vector. In this strict sense, the one-dimensional Doppler reduction does not survive configuration by configuration.

Nevertheless, the physical content of the reduction remains valid at the level relevant for mobility. The Volterra geometry of the dislocation (i.e., the fact that there exists a slip disregistry) is unchanged by chemical disorder, and the dislocation remains straight on average. The Kanzaki source therefore retains a strongly anisotropic structure in reciprocal space, with dominant weight concentrated near wave vectors parallel to the line direction. Disorder replaces the exact delta function constraints of the ordered case by narrow distributions whose width is controlled by the disorder correlation length and by the finite size of the atomistic region. For the long-wavelength modes that dominate the low-frequency sector of the spectral densities $\rho_n^C(\Omega)$ and hence the moments $B_{T,C}^{(n)}$, this broadening is parametrically small.

This observation underpins the construction adopted here. Rather than enforcing an exact one-dimensional reduction at the level of each configuration, we define the line-projected spectral densities $\rho_n^C(\Omega)$ as quadratic functionals of the Kanzaki source and the full retarded lattice response, without assuming Bloch structure or exact momentum conservation along the line. The moment functional $\kappa_{vC}^{(n)}$ introduced in Eq. (23) replaces the single Bloch wave number of the ordered case and captures the relevant line parallel content of each mode. In the ordered limit, this construction reduces identically to the exact Doppler form, while for disordered configurations it provides a well-defined and positive spectral measure for each order n .

Configurational averaging then restores the emergent symmetry of the problem. While $\rho_n^C(\Omega)$ fluctuates strongly between configurations, its ensemble average $\rho_n^{\text{HEA}}(\Omega)$ recovers a sharply defined line-projected spectral density that encodes both the Volterra geometry and the statistical effects of chemical disorder. The corresponding averaged kernels $\hat{\Gamma}_{T,\text{HEA}}^{(n)}(s)$ inherit the same Stieltjes structure and hierarchy as in the ordered theory, with the ordered spectral densities replaced by their disorder-averaged counterparts. In this sense, the one-dimensional character of the mobility kernel is not imposed but emerges naturally after averaging.

From a practical standpoint, two computational routes are available. If sufficiently large periodic supercells can be afforded, one may compute configuration-resolved quantities in the full supercell Brillouin zone and then project the resulting spectral weight onto effective line parallel components. In the limit of large transverse dimensions, this procedure converges to the isolated dislocation result, but its cost grows rapidly and

becomes prohibitive when force constants are obtained from expensive machine-learning models or *ab initio* methods.

The hybrid embedding approach adopted in Sec. VIC circumvents this difficulty. As we explain, we confine the disorder-induced breaking of translational invariance to a finite atomistic region that captures the Kanzaki vertex and local mode structure, while the far-field propagation is handled by an effective medium that restores translational invariance and corrects radiation conditions. In this formulation, the disorder-induced failure of exact Doppler reduction is localized and controlled, and the emergent one-dimensional structure is recovered after configurational averaging. The resulting disorder-averaged spectral densities $\rho_n^{\text{HEA}}(\Omega)$ are therefore the natural objects entering the mobility kernels and their moments, and form the starting point for the pole fitting and reduced mobility laws discussed in the following sections.

III. LIMITS OF HOMOGENEOUS EFFECTIVE MEDIA FOR PHONON DRAG IN DISORDERED ALLOYS

The discussion in the preceding Sec. IIE motivates a hybrid description in which the near-core region of the dislocation is treated explicitly for each chemical configuration, while the far-field lattice response is represented by an averaged effective medium. It is important to emphasize that this separation is not merely a matter of numerical convenience. A description based solely on a homogeneous effective medium, obtained by averaging the masses and force constants before constructing the dislocation–phonon coupling, fails to reproduce the correct phonon drag even in the thermodynamic limit. The reason is that the quantities controlling radiated power and mobility are nonlinear functionals of the Kanzaki source and of the lattice Green’s function. As a result, configurational averaging and the construction of an effective medium do not commute (q.v. Refs. [84,85]). In this section, we make this statement precise and clarify why the hybrid inner-region plus embedded-medium approach adopted here is the minimal framework consistent with the underlying Keldysh–Kanzaki theory.

To that end, consider a disordered alloy with a fixed chemical configuration C , site-dependent masses $M_C(\mathbf{R})$, and a harmonic force constant matrix $\Phi_{ij}^{(C)}(\mathbf{R}, \mathbf{R}')$. For a prescribed Volterra slip field $u_j^V(\mathbf{R}; X)$ representing a straight dislocation at position X , the Volterra Kanzaki force is defined by the linear response identity

$$f_i^V(\mathbf{R}; X; C) = - \sum_{\mathbf{R}', j} \Phi_{ij}^{(C)}(\mathbf{R}, \mathbf{R}') u_j^V(\mathbf{R}'; X). \quad (34)$$

The quantities that control radiated power and phonon drag are not linear in f^V . They depend on quadratic functionals such as $|g_{vC}|^2$, where g_{vC} is the projection of the source onto a normal mode v of configuration C , and more generally on bilinear forms $f^V \cdot \text{Im } G \cdot f^V$, where G is a retarded lattice Green’s function.

This is the origin of the nonequivalence between an averaged medium (see [45,86]) and an average over realizations. Define, for each C , a configuration-resolved spectral measure

$\rho_C(\Omega)$ such that the retarded memory kernel has Stieltjes form

$$\hat{\Gamma}_C(s) = s \int_0^\infty d\Omega \frac{\rho_C(\Omega)}{s^2 + \Omega^2}, \quad \text{Re } s > 0. \quad (35)$$

In a harmonic bath, $\rho_C(\Omega)$ is a positive measure built from squared couplings. In a mode representation, one may write schematically

$$\rho_C(\Omega) \propto \sum_v |g_{vC}|^2 \delta(\Omega - \omega_{vC}), \quad (36)$$

where the proportionality hides geometric factors such as line projections that are immaterial for the argument.

The disordered alloy kernel that enters a coarse-grained mobility law is the configurational average of the kernel, or equivalently of its spectral measure,

$$\hat{\Gamma}_{\text{HEA}}(s) = \langle \hat{\Gamma}_C(s) \rangle_C, \quad \rho_{\text{HEA}}(\Omega) = \langle \rho_C(\Omega) \rangle_C. \quad (37)$$

By contrast, an effective medium strategy that averages the lattice first replaces $\Phi^{(C)}$ and M_C by averaged objects $\bar{\Phi}$ and $\bar{M}$, then constructs a single kernel Γ_{eff} from that averaged medium. In a mode language, this corresponds to replacing the random couplings g_{vC} by some mean coupling $g_{v,\text{eff}}$, hence replacing $\langle |g_{vC}|^2 \rangle_C$ by $\langle |g_{vC}|^2 \rangle_C$ or by a similar mean field proxy. The distinction becomes explicit when one compares averaging before and after forming these quadratic couplings. Indeed, the discrepancy is then the variance term

$$\langle |g_{vC}|^2 \rangle_C = \langle |g_{vC}|^2 \rangle + \text{Var}_C(g_{vC}), \quad (38)$$

which is non-negative and generically nonzero in a chemically disordered alloy.

The additional contribution $\text{Var}_C(g_{vC})$ is precisely the disorder-induced enhancement of coupling strength that an averaged medium misses. The same point appears in the Green's function representation. For fixed C , radiated power and drag are controlled by objects of the form

$$\mathcal{P}_C \propto \int d\omega \omega f_C^V(\omega)^* \text{Im } G_C(\omega) f_C^V(\omega), \quad (39)$$

so that averaging produces $\langle f^* \text{Im } G f \rangle$, whereas replacing with an effective medium produces something closer to $\bar{f}^* \text{Im } \bar{G} \bar{f}$, with $\bar{f}$ constructed from $\bar{\Phi}$ and u^V . These are not equal because the average of a quadratic form of random fields is not the quadratic form of the averages. As will be discussed in Sec. VII, the magnitude of the variance $\text{Var}_C(g_{vC})$ contribution dominates the results by an order of magnitude or more, so that any effective medium theory will severely underestimate the magnitude of the dislocation drag.

There are several reasons for this. For one thing, the effective medium, the disorder is quenched, and one is comparing two different ensemble averages: an average of a nonlinear functional of C , and the value of that functional evaluated at an averaged operator. The noncommutativity is the familiar difference between quenched and annealed averaging of nonlinear observables [84,87]. In particular, even when the alloy is self-averaging in the thermodynamic limit, self-averaging applies to $\rho_{\text{HEA}}(\Omega) = \langle \rho_C(\Omega) \rangle_C$, not to the replacement $\rho_C(\Omega) \mapsto \rho_{\text{eff}}(\Omega)$ obtained by averaging the operator first. This is consistent with arguments made in the alloy lattice dynamics context that emphasize that force constant disorder enters through configuration-dependent spectral

functions and their disorder-induced broadening, and that naive homogenization misses essential fluctuation content [53,88].

The practical consequence is that an effective medium is appropriate for describing phonon propagation in the far field, where only averaged response functions enter, but it is not appropriate to replace the statistics of the Kanzaki source by a single averaged source. Retaining at least the second-moment information encoded in $\langle |g_{vC}|^2 \rangle_C$ is essential, and this is precisely what is achieved by resolving the disordered core region explicitly and performing configurational averaging only at the level of the resulting spectral measures.

IV. HYBRID EMBEDDING: ATOMISTIC KANZAKI CORE IN AN EFFECTIVE INFINITE MEDIUM

Chemically disordered alloys pose a structural obstruction to direct phonon drag calculations: for a fixed disorder realization C , the configuration-dependent harmonic operator $\Phi^{(C)}$ breaks translational invariance, so the lattice Green's function and the radiative boundary condition cannot be evaluated on length scales much larger than the atomistic supercell, as was done in chemically ordered systems in Ref. [71]. In principle, one could restore convergence by increasing the supercell until periodic images no longer contaminate the radiated spectrum, but this is computationally prohibitive when $\Phi^{(C)}$ is obtained from a machine-learned interatomic potential and must be recomputed for an ensemble of realizations. The hybrid embedding formulation resolves this by separating the problem into a disorder sensitive inner source region and a disorder-averaged far-field propagator, retaining the correct nonlinearity in the source statistics while enforcing outgoing radiation into an effectively infinite medium.

A. The embedding principle and block partition

Let $\mathcal{I}$ be a finite set of lattice degrees of freedom containing the slip plane and dislocation core, augmented by a buffer layer $\mathcal{B}$ of thickness several interaction ranges, and let $\mathcal{O}$ be its complement, treated as an infinite translationally invariant effective medium as in Fig. 2. For each disorder realization C restricted to $\mathcal{I}$, the full harmonic operator is partitioned as

$$\Phi(C) = \begin{pmatrix} \Phi_{\mathcal{II}}^{(C)} & \Phi_{\mathcal{IO}} \\ \Phi_{\mathcal{OI}} & \Phi_{\mathcal{OO}}^{\text{eff}} \end{pmatrix}, \quad M(C) = \begin{pmatrix} M_{\mathcal{I}}^{(C)} & 0 \\ 0 & M_{\mathcal{O}}^{\text{eff}} \end{pmatrix}, \quad (40)$$

where $\Phi_{\mathcal{II}}^{(C)}$ and $M_{\mathcal{I}}^{(C)}$ are extracted from the expensive atomistic model for the particular realization C , while $\Phi_{\mathcal{OO}}^{\text{eff}}$ and $M_{\mathcal{O}}^{\text{eff}}$ are deterministic and translationally invariant. The off-diagonal couplings $\Phi_{\mathcal{IO}}$ and $\Phi_{\mathcal{OI}}$ must be consistent with the lattice bookkeeping of the effective medium; in practice we take them from the effective medium operator so that the interface does not inherit configuration specific asymmetries that would otherwise generate uncontrolled ghost forces. The buffer $\mathcal{B} \subset \mathcal{I}$ is not an aesthetic refinement but the mechanism by which any residual impedance mismatch is rendered perturbative: the source support and the region in which $\Phi_{\mathcal{II}}^{(C)}$ differs strongly from Φ^{eff} are separated from the embedding boundary $\partial\mathcal{I}$ by a thickness large enough that the relevant

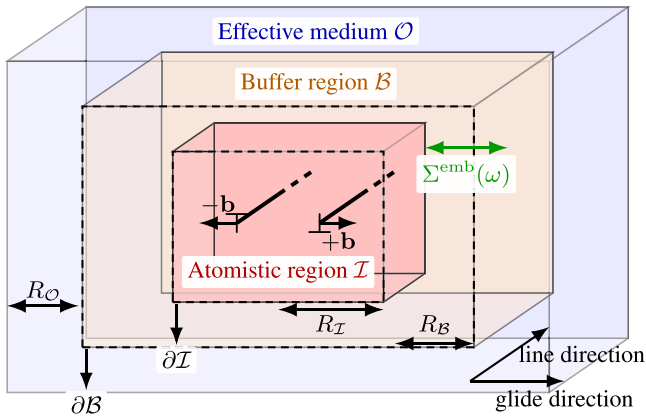


FIG. 2. Hybrid embedding geometry. The atomistic region $\mathcal{I}$ contains the dislocation dipole and supplies configuration-dependent Kanzaki data. The buffer $\mathcal{B}$ permits the atomistic distortion and any interface mismatch to decay before coupling to the translationally invariant effective medium $\mathcal{O}$. The embedding self-energy $\Sigma^{\text{emb}}(\omega)$ enforces outgoing radiation into $\mathcal{O}$.

evanescent components decay before reaching the interface, ensuring that spurious reflections are exponentially small at frequencies below the effective medium band edge [89,90].

The dislocation enters through a Kanzaki source supported in $\mathcal{I}$ and computed from the configuration-dependent inner operator. Using the Volterra representative $u^V(X)$ already fixed in Sec. II, we define the inner Volterra Kanzaki field by

$$f_{\mathcal{T}}^{\mathbf{V}}(X; C) = -\Phi_{\mathcal{T}\mathcal{T}}^{(C)} u_{\mathcal{T}}^{\mathbf{V}}(X), \quad (41)$$

with $u_{\mathcal{I}}^{\text{V}}$ the restriction of the same regularized Volterra field used in Eq. (3). This choice is the precise point at which disorder is retained in a way an effective medium alone cannot emulate: all observables relevant for drag are quadratic in the source and therefore depend on the second moment structure of $f_{\mathcal{I}}^{\text{V}}(X; C)$ and of its X derivatives, which must be sampled over C rather than replaced by a single averaged source. The outer region is not assigned an atomistic Kanzaki field; it enters only through its retarded propagator, whose role is to implement radiation into an infinite medium with the correct analytic structure.

Eliminating $\mathcal{O}$ by a Schur complement [91] yields an embedded resolvent on $\mathcal{I}$ that is exact for the composite operator defined by Eq. (40). Introducing the effective medium retarded Green's function

$$G_{\mathcal{O}\mathcal{O}}^{\text{eff}}(\omega) = [-\omega^2 M_{\mathcal{O}}^{\text{eff}} + \Phi_{\mathcal{O}\mathcal{O}}^{\text{eff}} + i0^+]^{-1}, \quad (42)$$

the embedding self-energy is

$$\Sigma^{\text{emb}}(\omega) = \Phi_{\mathcal{IO}} G_{\mathcal{OO}}^{\text{eff}}(\omega) \Phi_{\mathcal{OI}}, \quad (43)$$

and the embedded inner Green's function becomes

$$G_I^{\text{emb}}(\omega; C) = [-\omega^2 M_I^{(C)} + \Phi_{II}^{(C)} - \Sigma^{\text{emb}}(\omega) + i0^+]^{-1}. \quad (44)$$

Two analytic properties are essential for what follows and will be enforced explicitly in the numerical construction described in Sec. VI. First, $G_{\mathcal{O}\mathcal{O}}^{\text{eff}}$ must be a causal retarded resolvent of a mechanically stable operator, which implies $-\text{Im } G_{\mathcal{O}\mathcal{O}}^{\text{eff}}(\omega)$ is positive semidefinite for $\omega > 0$; this ensures that $\Sigma^{\text{emb}}(\omega)$

has the correct Herglotz structure, and that $-\operatorname{Im} G_{\mathcal{I}}^{\text{emb}}(\omega; C)$ is likewise positive semidefinite [92, 93]. Second, the mapping between the atomistic degrees of freedom in $\mathcal{I}$ and the lattice degrees of freedom underlying Φ^{eff} must be one-to-one, otherwise the interface coupling is ill posed, and the Schur complement construction does not represent any physical composite operator. These conditions are not optional technicalities but the algebraic prerequisites for the positivity of the spectral measure defined below.

B. Effective-medium dispersion and radiation

The effective medium Φ^{eff} is not introduced as an annealed substitute for quenched disorder, but as a deterministic propagator whose sole task is to impose correct far-field propagation and outgoing radiation [53]. Its construction must therefore satisfy translational invariance for computational tractability, mechanical stability so that $G_{\mathcal{O}\mathcal{O}}^{\text{eff}}(\omega)$ exists for $\omega > 0$, and fidelity to the long-wavelength elastic cone that controls the low-frequency sector of the drag kernel. In the strict $\omega \rightarrow 0$ limit, these requirements reduce to matching anisotropic elasticity. Writing C_{ijkl}^{eff} and ϱ^{eff} for the effective elastic constants and mass density of the alloy, the acoustic dispersion is

$$\omega_\alpha(\mathbf{q}) = c_\alpha(\hat{\mathbf{q}}) |\mathbf{q}| + o(|\mathbf{q}|), \quad (45)$$

$$C_{ijkl}^{\text{eff}} \hat{q}_j \hat{q}_l e_k^{(\alpha)} = \varrho^{\text{eff}} c_\alpha(\hat{\mathbf{q}})^2 e_i^{(\alpha)}, \quad (46)$$

so that the correct elastic anisotropy is encoded already at the level of the effective medium cone. This low-frequency sector is the one that controls the static drag $B = \hat{\Gamma}(0)$ and, more generally, the small s Stieltjes moments of $\hat{\Gamma}(s)$, hence it is the part of the spectrum where stability and bookkeeping errors most directly corrupt the final results.

At the same time, dislocation motion couples to a broad range of lattice frequencies once Doppler kinematics is taken into account [71], and the embedded formulation must provide a reasonable continuation beyond the elastic cone if one is to compute $\hat{\Gamma}(i\xi)$ on a bandwidth spanning grid for subsequent pole fitting [92]. For this purpose, Φ^{eff} is taken to be a lattice effective medium; that is, a translationally invariant force constant operator defined on the primitive cell of the underlying Bravais lattice and extended periodically. A practical and controlled construction is shell averaging: from a relaxed reference structure, one groups force constant blocks by relative lattice vector and basis indices, averages over equivalent pairs, and then reconstructs the on-site blocks by enforcing the acoustic sum rule exactly. This yields a stable lattice dynamical matrix $D^{\text{eff}}(\mathbf{q})$ that reproduces the correct anisotropic elastic cone as $\mathbf{q} \rightarrow 0$ while retaining branch structure and a physically reasonable density of states at intermediate $\mathbf{q}$. Once $D^{\text{eff}}(\mathbf{q})$ is fixed, $G_{\mathcal{O}\mathcal{O}}^{\text{eff}}(\omega)$ and hence $\Sigma^{\text{emb}}(\omega)$ can be evaluated efficiently by standard lattice Green’s function techniques, so the computational cost of representing an effectively infinite medium becomes negligible compared with the machine-learning interatomic potential (MLIP) cost of assembling $\Phi_{\tau\tau}^{(C)}$.

The conceptual separation is therefore sharp: disorder is kept where it enters through squared couplings and local core physics, while propagation is treated by an averaged, stable,

translationally invariant medium. This separation is precisely what fails if one attempts to use an effective medium alone, as discussed in Sec. III; the hybrid formulation should be read as the minimal modification that restores correct source statistics without surrendering the radiative boundary condition.

C. Power, spectral measures, and memory kernels in the embedded formulation

Once $G_{\mathcal{I}}^{\text{emb}}(\omega; C)$ is defined, all configuration-resolved dissipation quantities can be expressed as bilinear functionals of the inner source against the dissipative part of the embedded response. For a constant velocity protocol, the radiated power per unit length can be written in the generic quadratic form

$$P_C(v_d) = \frac{1}{2\pi} \int_0^\infty d\omega F_C(\omega; v_d)^* [-\text{Im } G_{\mathcal{I}}^{\text{emb}}(\omega; C)] F_C(\omega; v_d), \quad (47)$$

where $F_C(\omega; v_d)$ denotes the Fourier component of the generalized force conjugate to the collective coordinate, constructed from the Kanzaki source and Volterra geometry restricted to $\mathcal{I}$ in the same manner as in the full supercell theory. The role of the embedding is entirely contained in $G_{\mathcal{I}}^{\text{emb}}$: the imaginary part automatically encodes radiation into the infinite effective medium and, under the stability assumptions stated in Sec. IV A defines a positive quadratic form for every $\omega > 0$.

This positivity yields a direct construction of a configuration-resolved spectral measure for the retarded mobility kernel. Concretely, the line-projected spectral density entering the Stieltjes representation of Sec. II A admits an embedded counterpart $\rho_C^{\text{emb}}(\Omega)$ defined so that

$$\hat{\Gamma}_C^{\text{emb}}(s) = s \int_0^\infty d\Omega \frac{\rho_C^{\text{emb}}(\Omega)}{s^2 + \Omega^2}, \quad \text{Re } s > 0, \quad (48)$$

with $\rho_C^{\text{emb}}(\Omega) \geq 0$ by construction because it is built from overlaps against $-\text{Im } G_{\mathcal{I}}^{\text{emb}}(\Omega; C)$. In particular, the static drag extracted from the embedded kernel remains a genuine Stieltjes moment,

$$B_C^{\text{emb}} = \hat{\Gamma}_C^{\text{emb}}(0) = \int_0^\infty d\Omega \frac{\rho_C^{\text{emb}}(\Omega)}{\Omega}, \quad (49)$$

so the hybrid method preserves the same analytic structure as the exact theory, with the only modification being that the resolvent is computed with an embedded boundary condition rather than a periodically repeated supercell.

The high-entropy alloy objects are then obtained by configurational averaging at the level that is linear in the ensemble, namely, the kernels or, equivalently, their spectral measures,

$$\rho_{\text{HEA}}^{\text{emb}}(\Omega) = \langle \rho_C^{\text{emb}}(\Omega) \rangle_C, \quad (50)$$

$$\hat{\Gamma}_{\text{HEA}}^{\text{emb}}(s) = s \int_0^\infty d\Omega \frac{\rho_{\text{HEA}}^{\text{emb}}(\Omega)}{s^2 + \Omega^2}. \quad (51)$$

This is the unique averaging operation compatible with the linearity of the influence functional and with the fact that ρ_C is itself a nonlinear functional of C . It also yields the correct object for subsequent rational approximation: the pole fits used to build reduced mobility laws in Sec. VI H are performed on $\hat{\Gamma}_{\text{HEA}}^{\text{emb}}(i\xi)$, not on per-configuration fits, because only the former corresponds to an ensemble averaged kernel with a

well-defined Stieltjes structure. Per-configuration poles may still be extracted as diagnostics of local dynamical channels, but they are not averaged to obtain mobility parameters.

Finally, note that Fig. 2 uses a dipole geometry to suppress residual finite-size artifacts in the inner region and to provide internal consistency checks through self- and cross-dissipation; the precise relation between dipole observables and the single-dislocation kernel is not a minor technicality and is therefore developed separately in Sec. V, where the matrix-valued kernel structure and the projection relations are established rigorously. The specifics of the computational implementation of this protocol are discussed in Sec. VI.

V. DIPOLE PROTOCOL AND RECOVERY OF THE SINGLE-DISLOCATION DRAG

The embedded implementation of Sec. IV uses a dislocation dipole rather than an isolated line. This is not merely a computational convenience but a structural requirement: a single dislocation in a finite inner region $\mathcal{I}$ produces a net Burgers vector that must be screened by image contributions from $\mathcal{O}$, coupling the result to artifacts of the embedding boundary. A dipole of zero net Burgers vector has a faster decaying far field and can be contained within $\mathcal{I}$ with the distortion already small at $\partial\mathcal{I}$, so that the embedding interface samples an essentially elastic field rather than a singular core. The cost of this regularization is that the object directly accessible from the embedded power integral is not the single-dislocation drag but a bilinear form over the two lines, containing both self and cross-dissipation. This section establishes the matrix structure of the two-line kernel, derives the projection that produces the dipole observable returned by the calculation, and identifies conditions under which cross-dissipation is negligible so that the single-dislocation drag is recovered in a controlled manner.

A. Matrix-valued spectral measures and retarded kernels for two lines

Consider two straight dislocations labeled $a \in \{1, 2\}$ with glide coordinates $X_a(t)$ and fixed transverse separation d within $\mathcal{I}$. For a fixed configuration C , each line has an associated Kanzaki coupling to the embedded phonon spectrum. Generalizing Eq. (22) to the two-line case, define

$$C_{vC,a} = -\sqrt{\frac{\hbar}{2M_{\text{ref}}\omega_{vC}}} \sum_{\mathbf{R},i} [\partial_{X_a} f_i^K(\mathbf{R}; X_a; C)] e_i^{(vC)}(\mathbf{R}), \quad (52)$$

where $\partial_{X_a} f^K$ is the derivative of the Kanzaki force with respect to the glide coordinate of line a . Replacing $|C_{vC}|^2$ in Eq. (23) by the outer product $C_{vC,a}^* C_{vC,b}$ yields a matrix of line-projected spectral measures

$$\rho_{n,ab}^C(\Omega) = \frac{\hbar}{Q} \sum_v \frac{\kappa_{vC}^{(n)}}{n!} \frac{C_{vC,a}^* C_{vC,b}}{\omega_{vC}} \delta(\Omega - \omega_{vC}), \quad (53)$$

where $n = 0, 1, 2, \dots$, and $\kappa_{vC}^{(n)}$ is the line-projection moment defined in Sec. II. For each fixed Ω , the matrix $\rho_n^C(\Omega) = [\rho_{n,ab}^C(\Omega)]_{a,b=1}^2$ is Hermitian and positive semidefinite, since it is a sum of rank-one matrices $C_{vC} C_{vC}^*$ with non-negative

weights $(\kappa_{nC}/n! \omega_{nC}) \geq 0$. Equivalently, $\eta^* \rho_n^C(\Omega) \eta \geq 0$ for all $\eta \in \mathbb{C}^2$, which guarantees that all quadratic forms constructed from ρ_n^C yield non-negative dissipation, as required for a passive harmonic bath.

The corresponding matrix of retarded memory kernels is

$$\hat{\Gamma}_{C,ab}^{(n)}(s) = s \int_0^\infty d\Omega \frac{\rho_{n,ab}^C(\Omega)}{s^2 + \Omega^2}, \quad \text{Re } s > 0. \quad (54)$$

In the present harmonic setting with linear coupling, $\rho_{n,ab}^C$ and $\hat{\Gamma}_{C,ab}^{(n)}$ are purely mechanical objects, determined by the harmonic operators and Kanzaki vertices, and independent of temperature. Thermal effects enter only through the Keldysh sector (noise kernel) via the Bose factor in the fluctuation-dissipation relation in Sec. II.

In the linear-mobility regime, the relevant coefficient matrix is the $n = 1$ static limit:

$$B_{C,ab}^{(1)} \equiv \hat{\Gamma}_{C,ab}^{(1)}(0), \quad (55)$$

so that a constant velocity protocol $X_a(t) = v_a t$ yields configuration-resolved dissipation in quadratic form

$$P^{(C)}(\{v_a\}) = \sum_{a,b} v_a v_b B_{C,ab}^{(1)}. \quad (56)$$

The single-dislocation drag in configuration C is given by one of the diagonal entries $B_{C,11}^{(1)}$ or $B_{C,22}^{(1)}$, whereas the dipole computation returns a particular projection of the full matrix $B_C^{(1)}$.

B. Projection onto the dipole channel

A dipole protocol constrains the two lines to glide together with a single collective coordinate $X(t)$, while their Kanzaki sources enter with opposite topological signs. Concretely, we introduce a sign vector $\sigma = (\sigma_1, \sigma_2)$ with $\sigma_a = \pm 1$ and $\sigma_1 + \sigma_2 = 0$, so that the composite source is $f_{\text{dip}}^K = \sigma_1 f_1^K + \sigma_2 f_2^K$. The sign vector σ is fixed by the Volterra topology of the two cores and encodes the relative orientation of the Burgers vectors, independently of any kinematic choice for the glide velocities.

At the level of mode couplings, this induces $C_{vC}^{\text{dip}} = \sigma_1 C_{vC,1} + \sigma_2 C_{vC,2}$, and all quadratic observables inherit the same projection. In particular, the dipole spectral measure and kernel are

$$\rho_n^{C,\text{dip}}(\Omega) = \sum_{a,b} \sigma_a \sigma_b \rho_{n,ab}^C(\Omega), \quad (57)$$

and

$$\hat{\Gamma}_C^{(n),\text{dip}}(s) = \sum_{a,b} \sigma_a \sigma_b \hat{\Gamma}_{C,ab}^{(n)}(s). \quad (58)$$

For the physical opposite-sign dipole $\sigma = (+1, -1)$, the projected drag coefficient is

$$B_C^{(1),-} = B_{C,11}^{(1)} + B_{C,22}^{(1)} - 2B_{C,12}^{(1)}. \quad (59)$$

The two self terms need not coincide for a fixed C in a disordered alloy, because the two cores sample different local chemical environments. The cross term $B_{C,12}^{(1)}$ encodes dissipation arising from coherent excitation of lattice modes by both cores simultaneously, so that the dipole observable is a

specific linear combination of three independent quantities, not a direct measurement of either self-drag.

If one also computes the same-sign projection $\sigma_+ = (+1, +1)$, then

$$B_C^{(1),+} = B_{C,11}^{(1)} + B_{C,22}^{(1)} + 2B_{C,12}^{(1)},$$

$$B_C^{(1),-} = B_{C,11}^{(1)} + B_{C,22}^{(1)} - 2B_{C,12}^{(1)}, \quad (60)$$

and self- and cross-contributions can be recovered algebraically:

$$B_{C,11}^{(1)} + B_{C,22}^{(1)} = \frac{1}{2}(B_C^{(1),+} + B_C^{(1),-}), \quad (61)$$

$$B_{C,12}^{(1)} = \frac{1}{4}(B_C^{(1),+} - B_C^{(1),-}). \quad (62)$$

The same projection logic applies to the full Laplace-domain kernels $\hat{\Gamma}_{C,ab}^{(n)}(s)$ via Eq. (58).

C. Disorder averaging and conversion to single-line drag

To fix conventions unambiguously, we define the projected dipole coefficient by the identity

$$P^{(C)}(v) = v^2 B_C^{(1),-}, \quad (63)$$

where $X(t) = vt$ is the single collective coordinate used in the dipole calculation and $B_C^{(1),-}$ is given by Eq. (59). Under this definition, $B_C^{(1),-}$ is a per-dipole quantity, in the sense that it accounts for the total dissipation of both lines. The corresponding per-line normalization is therefore $B_{C,\text{per line}}^{(1),-} \equiv \frac{1}{2} B_C^{(1),-}$.

Introduce an ensemble over configurations C in which the two line positions are treated symmetrically. Then $B_{C,11}^{(1)}$ and $B_{C,22}^{(1)}$ are exchangeable random variables and satisfy

$$\langle B_{C,11}^{(1)} \rangle_C = \langle B_{C,22}^{(1)} \rangle_C = \frac{1}{2} \langle B_{C,11}^{(1)} + B_{C,22}^{(1)} \rangle_C. \quad (64)$$

If, in addition, the averaged cross-dissipation is negligible,

$$|\langle B_{C,12}^{(1)} \rangle_C| \ll \langle B_{C,11}^{(1)} \rangle_C, \quad (65)$$

then Eq. (59) implies $\langle B_C^{(1),-} \rangle_C \simeq 2 \langle B_{C,11}^{(1)} \rangle_C$, hence

$$\langle B_{C,11}^{(1)} \rangle_C \simeq \frac{1}{2} \langle B_C^{(1),-} \rangle_C, \quad \langle B_{C,11}^{(1)} \rangle_C \simeq \langle B_{C,\text{per line}}^{(1),-} \rangle_C. \quad (66)$$

Any other prefactor arises only from a different reporting convention upstream. In this work, we fix the convention by Eq. (63) and use Eq. (66) throughout.

D. Coherence criterion and separation estimates

The validity of Eq. (65) depends on the separation d between the two cores and on the coherence properties of the embedded dissipative propagator. In the embedded formulation, the drag matrix elements may be written as overlaps:

$$B_{C,ab}^{(1)} = \frac{1}{2\pi} \int_0^\infty d\omega \omega F_{a,C}(\omega)^* [-\text{Im } G_T^{\text{emb}}(\omega; C)] F_{b,C}(\omega), \quad (67)$$

where $F_{a,C}(\omega)$ is the Fourier transform of the effective driving force conjugate to X_a , restricted to $\mathcal{I}$. Since $-\text{Im } G_T^{\text{emb}}(\omega; C)$ is positive semidefinite for each $\omega > 0$, it defines a positive

sesquilinear form, hence an ω -dependent inner product. Define the positive spectral weight

$$\mathcal{W}_C(\omega) \equiv \frac{1}{2\pi} \omega F_{1,C}(\omega)^* [-\text{Im } G_{\mathcal{I}}^{\text{emb}}(\omega; C)] F_{1,C}(\omega), \quad (68)$$

so that $B_{C,11}^{(1)} = \int_0^\infty d\omega \mathcal{W}_C(\omega)$, and the normalized coherence factor

$$\mathcal{C}_C(\omega; d) \equiv \frac{F_{1,C}(\omega)^* [-\text{Im } G_{\mathcal{I}}^{\text{emb}}(\omega; C)] F_{2,C}(\omega)}{F_{1,C}(\omega)^* [-\text{Im } G_{\mathcal{I}}^{\text{emb}}(\omega; C)] F_{1,C}(\omega)}. \quad (69)$$

Cauchy–Schwarz in the inner product induced by $-\text{Im } G_{\mathcal{I}}^{\text{emb}}$ gives $|\mathcal{C}_C(\omega; d)| \leq 1$ for all ω , while the phase of $\mathcal{C}_C$ encodes whether the two cores radiate predominantly in phase or out of phase at that frequency.

The cross-dissipation is then

$$B_{C,12}^{(1)} = \int_0^\infty d\omega \mathcal{W}_C(\omega) \mathcal{C}_C(\omega; d). \quad (70)$$

In a chemically disordered alloy, $\mathcal{C}_C(\omega; d)$ decays with d because line-parallel components excited by one core suffer dephasing from disorder-broadened $k_{\parallel}$ content and, when $\gamma(\omega; C) > 0$, attenuation from finite vibrational lifetimes. A convenient envelope capturing both effects is

$$|\mathcal{C}_C(\omega; d)| \lesssim \exp[-d/\ell_{\text{coh}}(\omega; C)], \quad (71)$$

which should be read as an effective bound once either spectral broadening or a finite linewidth renders the ω integral self-averaging. In the purely ballistic limit $\gamma \rightarrow 0$ the suppression is controlled by oscillatory phase cancellation (stationary-phase decay), but for broadband $\mathcal{W}_C$ this leads to the same practical conclusion that cross-dissipation becomes small beyond a moderate separation.

A useful estimate for the coherence length is

$$\ell_{\text{coh}}(\omega; C) \simeq \min \left\{ \frac{1}{\Delta k_{\parallel}(\omega; C)}, \frac{v_g(\omega; C)}{2\gamma(\omega; C)} \right\}, \quad (72)$$

where $\Delta k_{\parallel}$ is the disorder-broadened width of the line-parallel wave number content at frequency ω , v_g is the relevant group velocity along the slip direction, and γ is the disorder-induced vibrational linewidth.

To convert this frequency-dependent estimate into a practical criterion, define a representative frequency ω_* by the centroid of weight

$$\omega_* \equiv \frac{\int_0^\infty d\omega \omega \mathcal{W}_C(\omega)}{\int_0^\infty d\omega \mathcal{W}_C(\omega)}. \quad (73)$$

A sufficient condition for negligible cross-dissipation is then $d \gg \ell_{\text{coh}}(\omega_*)$, in which case $|\langle B_{C,12}^{(1)} \rangle_C| / \langle B_{C,11}^{(1)} \rangle_C$ is small and Eq. (66) applies.

For a concrete estimate, inelastic x-ray scattering in the Cantor alloy FeCoCrMnNi resolves strong disorder scattering with a characteristic length of order 10 Å, in the sense that the transition from ballistic to diffusive phonon transport occurs on the scale of one to two lattice spacings [94]. Interpreting this as $\ell_{\text{coh}}(\omega_*) \approx 1$ nm at representative frequencies, the cross-dissipation is suppressed to a few percent once $d \gtrsim 3 \ell_{\text{coh}} \approx 3$ nm, since $\exp(-3) \approx 0.05$. A conservative choice is $d \approx 5$ nm. This estimate applies to the portion of the spectrum where disorder broadening is experimentally

resolved; linewidths below approximately 10 meV are not resolved and correspond to longer mean-free paths, which would increase the required d if $\mathcal{W}_C$ were concentrated predominantly at such low energies.

In practice, the regime of negligible cross-dissipation can be verified without estimating ℓ_{coh} explicitly. A separation sweep showing saturation of $\langle B_C^{(1),-}(d) \rangle_C$ with increasing d indicates that cross-dissipation is no longer influencing the observable. Alternatively, computing both projections $\sigma_{\pm}$ at fixed d and observing $\langle B_C^{(1),+} \rangle_C \simeq \langle B_C^{(1),-} \rangle_C$ implies $\langle B_{C,12}^{(1)} \rangle_C \simeq 0$ through Eq. (62).

VI. COMPUTATIONAL IMPLEMENTATION

The hybrid embedding formulation of Sec. IV and the dipole protocol of Sec. V reduce the computation of disorder-averaged dislocation drag to a sequence of well-defined numerical operations. The purpose of this section is not merely to list those operations, but to make explicit which steps are logically essential, which are numerical conveniences, and which failure modes invalidate the construction irrespective of the fidelity of the underlying force constants.

A recurring theme is that the embedded Green's function represents a passive harmonic bath. Mechanical instability, bookkeeping ambiguity, or improper interface construction destroy passivity and therefore invalidate the Stieltjes structure of the memory kernel. The implementation must be organized to prevent such pathologies by construction rather than by posterior filtering.

A. Overview of the computational pipeline

The calculation separates naturally into three layers, ordered by increasing configuration dependence.

First, a translationally invariant effective medium operator Φ^{eff} is constructed once from a relaxed reference supercell by shell averaging and exact enforcement of the acoustic sum rule. This operator defines the far-field propagator and radiation condition and is reused unchanged throughout the calculation.

Second, an ensemble of configuration-dependent inner problems is generated. For each disorder realization C on the inner region $\mathcal{I}$, atomic positions and cell degrees of freedom are fully relaxed under the interatomic force field (or *ab initio* method) of choice, the configuration-dependent inner force constants $\Phi_{\mathcal{I}\mathcal{I}}^{(C)}$ are extracted, and the Kanzaki forcing associated with a dislocation dipole is constructed. This stage dominates the computational cost.

Third, for each C , the embedded Green's function $G_{\mathcal{I}}^{\text{emb}}(\omega; C)$ is assembled, the dipole projected spectral density $\rho_C^{\text{emb}}(\Omega)$ is evaluated, and these spectral measures are averaged over configurations to obtain the HEA kernel $\hat{\Gamma}_{\text{HEA}}^{\text{emb}}(s)$.

The geometry follows Fig. 2. The inner region $\mathcal{I}$ contains both dislocation cores and a buffer region $\mathcal{B}$ of several interaction ranges. The core separation d satisfies the coherence criterion of Sec. V D, while the buffer ensures that the Kanzaki forcing and its glide derivatives are negligible at the embedding interface before coupling to the effective medium.

B. Relaxation and mechanical stability

Every harmonic operator appearing in this work is the Hessian of the potential energy evaluated at a mechanically stationary configuration [95]. This requirement is structural: if the reference configuration is not a local minimum with respect to both atomic positions and cell degrees of freedom, the resulting force constant matrix does not define a stable harmonic bath and the retarded Green's function ceases to be well-defined.

For each configuration C , atomic positions and supercell vectors are relaxed at zero temperature under the interatomic force field of choice. Only after relaxation are harmonic force constants computed by central finite differences using displacements $\delta \approx 0.01 \text{ \AA}$, small enough to suppress anharmonic contributions while remaining robust to numerical noise [96].

The acoustic sum rule is then enforced on $\Phi_{\mathcal{II}}^{(C)}$ by adjusting on-site blocks so that

$$\sum_{\mathbf{R}', j} \Phi_{ij}^{(C)}(\mathbf{R}, \mathbf{R}') = 0, \quad (74)$$

for each $\mathbf{R} \in \mathcal{I}$ and Cartesian index i . This guarantees exact translational invariance of the inner operator.

In chemically disordered alloys, this step is indispensable (cf. Ref. [97]). An unrelaxed random or SQS structure is generically far from equilibrium, and its curvature describes a saddle rather than a basin. Force constants extracted from such a configuration exhibit large negative eigenvalues unrelated to any physical instability and render the embedded response meaningless.

Configurations that retain negative eigenvalues beyond the three translational zero modes after relaxation and sum-rule enforcement are excluded from the ensemble. Within the present framework, the bath is harmonic and passive; genuine mechanical instabilities would require an explicitly anharmonic or nonequilibrium treatment and therefore lie outside the scope of the kernel construction.

C. Construction of the effective medium

The effective medium Φ^{eff} is a translationally invariant harmonic operator whose sole role is to propagate elastic radiation away from the inner region with the correct long-wavelength structure [53]. It is not intended to reproduce local disorder physics.

Starting from a relaxed reference supercell, force constant blocks are assigned lattice cell indices $\mathbf{R}_{\text{lat}}$ and basis indices b using the bookkeeping procedure described in Sec. VID. Blocks are grouped by relative lattice vector $\mathbf{d} = \mathbf{R}'_{\text{lat}} - \mathbf{R}_{\text{lat}}$ and basis pair (b, b') and averaged to obtain shell matrices $\Phi_{bb'}^{\text{eff}}(\mathbf{d})$.

The on-site blocks are reconstructed by enforcing the acoustic sum rule exactly [98,99],

$$\Phi_{bb}^{\text{eff}}(\mathbf{0}) = - \sum_{\mathbf{d} \neq \mathbf{0}} \sum_{b'} \Phi_{bb'}^{\text{eff}}(\mathbf{d}), \quad (75)$$

and Hermiticity is enforced by explicit symmetrization,

$$\Phi_{bb'}^{\text{eff}}(\mathbf{d}) \rightarrow \frac{1}{2} [\Phi_{bb'}^{\text{eff}}(\mathbf{d}) + \Phi_{b'b}^{\text{eff}T}(-\mathbf{d})]. \quad (76)$$

The resulting lattice dynamical matrix $D^{\text{eff}}(\mathbf{q})$ must exhibit exactly three zero modes at $\mathbf{q} = \mathbf{0}$ and no negative eigenvalues

on a verification mesh. This check is mandatory, because $G_{\mathcal{OO}}^{\text{eff}}(\omega)$ enters the embedding self-energy as a retarded propagator.

The effective medium-mass matrix is diagonal with basis masses [53],

$$M_b^{\text{eff}} = \sum_{\alpha} c_{\alpha} m_{\alpha}, \quad (77)$$

ensuring that the continuum limit reproduces the correct elastic wave speeds.

D. Lattice bookkeeping and site identification

A consistent embedding requires a bijection between atoms in $\mathcal{I}$ and lattice degrees of freedom of the effective medium. This bijection defines the meaning of $\Phi_{\mathcal{IO}}$ and $\Phi_{\mathcal{OI}}$ in Eq. (40).

Each atomic position $\mathbf{r}$ is decomposed as

$$\mathbf{r} = \sum_i n_i \mathbf{a}_i + \boldsymbol{\tau}_b + \boldsymbol{\delta}, \quad (78)$$

with $(n_1, n_2, n_3) \in \mathbb{Z}^3$, basis index b , and residual displacement $|\boldsymbol{\delta}| < r_{\text{cut}}$. The cutoff must be smaller than half the minimum basis separation to ensure uniqueness. Any violation of bijectivity indicates a bookkeeping failure and invalidates the interface construction.

This requirement is particularly stringent for noncubic orientations and nonstandard dislocation geometries, where naive Cartesian rounding fails.

E. Interface coupling and the role of the buffer

The interface blocks $\Phi_{\mathcal{IO}}$ and $\Phi_{\mathcal{OI}}$ are constructed exclusively from the effective medium shells,

$$\Phi_{ij}(\mathbf{R}, \mathbf{R}') = [\Phi_{bb'}^{\text{eff}}(\mathbf{R}'_{\text{lat}} - \mathbf{R}_{\text{lat}})]_{ij}, \quad (79)$$

with Hermiticity enforcing $\Phi_{\mathcal{OI}} = \Phi_{\mathcal{IO}}^T$.

This replacement introduces an approximation: true configuration-dependent couplings across $\partial\mathcal{I}$ are replaced by averaged ones. The buffer region $\mathcal{B}$ is introduced precisely to control this approximation (q.v. Refs. [89,90,100,101]). Its purpose is not to represent physics, but to ensure that the Kanzaki forcing $\partial_{\mathbf{x}_a} f^K$ has decayed to numerical zero before the embedding interface. Since the projected driving fields $F_{a,C}(\omega)$ depend only on these sources, errors introduced by averaging at the interface are exponentially small in the buffer thickness for frequencies below the effective medium bandwidth.

F. Outer Green function and recursive decimation

The outer Green's function $G_{\mathcal{OO}}^{\text{eff}}(\omega)$ must be evaluated for a semi-infinite effective medium with outgoing radiation boundary conditions [89,90]. Direct inversion is not feasible because the outer region $\mathcal{O}$ is infinite. For a translationally invariant medium, however, the problem admits an efficient recursive solution.

The key observation is that a semi-infinite harmonic lattice can be partitioned into principal layers normal to the embedding surface, each layer interacting only with its nearest neighbors. In the present geometry, the dislocation line

direction is retained as periodic while the two transverse directions are left open, so the outer region is not a single semi-infinite chain but a laterally infinite medium. The outer Green's function is accordingly evaluated as the bulk lattice Green's function of the effective medium, $G_{\mathcal{O}\mathcal{O}}^{\text{inf}}(\omega) = \mathcal{F}^{-1}([\omega^2 M - K(\mathbf{q})]^{-1})$, with $\omega \rightarrow \omega + i0^+$, obtained by fast Fourier transform of the inverse dynamical matrix over a fine transverse Brillouin-zone mesh at each frequency. If H_0 denotes the intralayer dynamical matrix block and H_1 the interlayer coupling, then the surface Green's function $g_0(\omega)$ satisfies a self-consistent equation involving the bulk Green's function of the remaining semi-infinite chain [102]. Rather than solving this equation by direct iteration, which converges slowly near band edges and at low frequencies, we verified against the Sancho-Rubio decimation algorithm [103]. The decimation is recovered as the one open direction limit of this construction, in which a single surface is exposed, and the remaining directions are periodic, and we retain it as an independent correctness gate against which the bulk lattice Green's function embedding is verified.

The Sancho-Rubio decimation proceeds by iteratively eliminating every second layer, renormalizing the effective intralayer and interlayer couplings at each step. After n iterations, the effective coupling spans 2^n original layers, and the renormalized interlayer term $H_1^{(n)}$ decays geometrically. Convergence is monitored by tracking $\|H_1^{(n)}\|$; when this falls below a specified tolerance, the surface Green's function is extracted from the accumulated self-energy. The algorithm is numerically stable and converges in $O(\log N)$ iterations for a chain of N layers, making it well-suited to the present application where $G_{\mathcal{O}\mathcal{O}}^{\text{eff}}(\omega)$ must be evaluated at approximately 10^3 frequencies.

The embedding self-energy $\Sigma^{\text{emb}}(\omega)$ is then assembled as in Eq. (43). For each configuration C , the embedded inner Green's function $G_{\mathcal{I}}^{\text{emb}}(\omega; C)$ is constructed via Eq. (44) and inverted on a frequency grid dense enough to resolve the spectral features entering the drag kernel. The evaluation is performed on both the real axis $\omega + i0^+$, which yields the spectral density, and the positive imaginary axis $i\xi$, which is used for the rational approximation described in Sec. VIH.

G. Spectral densities and averaging

For each configuration, the dipole projected spectral density is computed as

$$\rho_C^{\text{emb}}(\Omega) = \frac{1}{\pi} F_{\text{dip},C}^*(\Omega) [-\text{Im } G_{\mathcal{I}}^{\text{emb}}(\Omega; C)] F_{\text{dip},C}(\Omega), \quad (80)$$

where $F_{\text{dip},C}(\Omega) = \sum_a \sigma_a F_{a,C}(\Omega)$ is the dipole-projected driving force constructed from the Fourier-transformed Kanzaki forces of the two lines, with sign vector $\sigma = (+1, -1)$ as defined in Sec. VB. Positivity of $\rho_C^{\text{emb}}(\Omega)$ for all $\Omega > 0$ is a stringent diagnostic of correctness: any negative value indicates a failure of mechanical stability, bookkeeping, or sum-rule enforcement upstream.

Averaging over configurations yields $\rho_{\text{HEA}}^{\text{emb}}(\Omega) = \langle \rho_C^{\text{emb}}(\Omega) \rangle_C$ and the kernel

$$\hat{\Gamma}_{\text{HEA}}^{\text{emb}}(s) = s \int_0^\infty \frac{\rho_{\text{HEA}}^{\text{emb}}(\Omega)}{s^2 + \Omega^2} d\Omega. \quad (81)$$

The static drag coefficient is

$$B_{\text{HEA}}^{\text{emb}} = \hat{\Gamma}_{\text{HEA}}^{\text{emb}}(0) = \int_0^\infty \frac{\rho_{\text{HEA}}^{\text{emb}}(\Omega)}{\Omega} d\Omega. \quad (82)$$

Consistency between the real-axis and imaginary-axis evaluations is monitored by verifying that $B_{\text{HEA}}^{\text{emb}}$ obtained from the Stieltjes integral over $\rho_{\text{HEA}}^{\text{emb}}$ agrees with the $\xi \rightarrow 0$ limit of $\hat{\Gamma}_{\text{HEA}}^{\text{emb}}(i\xi)$ evaluated directly on the imaginary axis. Discrepancies beyond numerical tolerance indicate inadequate frequency resolution or interpolation error.

H. Rational approximation for mesoscale dynamics

The general mobility law for a dislocation entailed by Eq. (15) is

$$b\tau_{\text{RSS}}(t) = \int_0^t \hat{\Gamma}_{\text{HEA}}(t - t') \dot{X}(t') dt' \quad (83)$$

where τ_{RSS} is the resolved shear stress acting on the dislocation. Although it is possible to compute the full ensemble averaged nonlocal memory kernel in real space, $\hat{\Gamma}_{\text{HEA}}$ (and indeed, all calculations we report in Sec. VIIC rely on so doing), it is inherently a numerical entity.

For mesoscale dislocation dynamics or crystal plasticity, it is possible to approximate the nonlocal kernel $\hat{\Gamma}_{\text{HEA}}^{\text{emb}}(s)$ to great accuracy by a rational Stieltjes form,

$$\hat{\Gamma}_{\text{HEA}}^{\text{emb}}(s) \simeq \sum_{m=1}^{N_{\text{poles}}} \frac{w_m \Omega_m^2}{s^2 + \Omega_m^2}, \quad w_m > 0, \quad \Omega_m > 0, \quad (84)$$

which preserves causality, passivity, and complete monotonicity by construction [104].

The fit of $\hat{\Gamma}_{\text{HEA}}^{\text{emb}}$ to its Stieltjes form must be performed on the averaged kernel evaluated on the positive imaginary axis, where $\hat{\Gamma}_{\text{HEA}}^{\text{emb}}(i\xi)$ is real and well conditioned. Positivity of the weights and strict ordering of the poles are enforced, together with the static moment constraint [105]

$$\sum_{m=1}^{N_{\text{poles}}} w_m = B_{\text{HEA}}^{\text{emb}}, \quad (85)$$

ensuring exact recovery of the atomistically determined drag coefficient.

The rational form in Eq. (84) corresponds to an oscillatory causal kernel and is realized in the time domain through second-order auxiliary variables $\{q_m, p_m\}_{m=1}^{N_{\text{poles}}}$ [106],

$$\dot{q}_m = p_m, \quad \dot{p}_m = -\Omega_m^2 q_m + \Omega_m^2 v, \quad F_{\text{drag}} = \sum_{m=1}^{N_{\text{poles}}} w_m q_m, \quad (86)$$

with vanishing initial data $q_m(0) = p_m(0) = 0$ unless a velocity prehistory is prescribed. Eliminating $\{q_m, p_m\}$ via Laplace transform recovers $F_{\text{drag}}(s) = \hat{\Gamma}_{\text{HEA}}^{\text{emb}}(s) v(s)$ with $\hat{\Gamma}_{\text{HEA}}^{\text{emb}}$ given by Eq. (84). This representation avoids explicit convolution over the velocity history and introduces $2N_{\text{poles}}$ internal degrees of freedom per dislocation segment.

The number of poles controls a transparent trade-off between fidelity and computational cost. In practice, $N_{\text{poles}} \approx 1-2$ captures the dominant relaxation physics over

temporal scales accessible to, i.e., MD, while a larger number of poles yields quantitative agreement across the full vibrational bandwidth, providing information concerning femto and subfemtosecond timescales.

Physical interpretation of the poles. The pole representation of the mobility kernel is best understood as a reduced-order surrogate of the exact spectral representation, not as a decomposition into microscopic excitations and preferential dissipative timescales. The kernel $\hat{\Gamma}(s)$ is a Stieltjes function determined by the positive projected spectral measure induced by the Kanzaki vertex. The approximation in Eq. (84) replaces this continuum measure by a discrete measure with nodes $\{\Omega_m\}$ and weights $\{w_m\}$, constructed so that causality and passivity are preserved and $\hat{\Gamma}(s)$ is reproduced over the Laplace frequency range relevant for dislocation motion. For this reason, the fitted poles are not material constants, nor do they define proper intrinsic dissipative timescales of the lattice. They are quadrature nodes of the Kanzaki projected spectrum, and the associated weights are the corresponding quadrature weights that encode how the dislocation samples the harmonic degrees of freedom.

Within this interpretation, the slowest pole represents the dominant low-frequency contribution of the projected measure and therefore controls the long-time tail of $\Gamma(t)$ together with the static drag. The remaining poles provide a compact aggregation of the residual spectral weight needed to represent the finite frequency response, so that the memory kernel is faithfully captured with a minimal number of effective relaxation components. The success of one or two poles across the systems considered should therefore be read in terms of the successful encapsulation of the whole kernel over the relevant dynamical band and timescale, rather than as evidence for a small set of distinct microscopic damping mechanisms or timescales.

This is because, physically, the dissipation is distributed across the entire projected spectrum because the drag is an integral functional. Unless the projected spectral measure contains an actual narrow peak, there is no distinguished frequency at which dissipation takes place: dissipation in dislocation motion is an accumulated effect of many modes weighted by the Kanzaki coupling and by the resolvent. Furthermore, the inverse problem is ill-conditioned: many different discrete measures, hence many different pole sets, produce nearly indistinguishable kernels on the timescales relevant for glide. High-frequency poles in particular only affect the kernel at very short timescales, so if the data and regime of interest do not resolve the initial boundary layer (as is the case in, i.e., MD style dynamics, where the time step is of order of a femtosecond, and therefore cannot capture dissipative over such timescales), those poles are not identifiable and will drift with discretization and regularization.

Thus, the poles fitted here supply a numerically convenient parametrization of the hereditary mobility law on experimentally relevant timescales, while the underlying physical content remains the full projected spectral measure that enters the exact Stieltjes representation. They are not physical constants, and should not be read as such. A more physically insightful but less accurate representation of dislocation dissipative channels is provided by the moment hierarchy introduced in [71]; here we favor the Stieltjes representation as

a more accurate representation of the dynamics of dislocation motion over the relevant timescales.

VII. DISLOCATION MOBILITY IN DISORDERED SYSTEMS

Sections II–V show that the phonon-mediated drag of a straight gliding dislocation is governed, at reduced order, by a causal memory kernel with a Stieltjes representation. Section VI specifies the embedded computation of the configuration-resolved kernels in a chemically disordered alloy and their conversion from a dipole observable to a single-line quantity. The purpose of the present section is to fix the bookkeeping required for mesoscale mobility laws and to justify, under explicit hypotheses, the use of a stationary ensemble-averaged kernel to represent the drag experienced by a single line as it traverses many local environments. We apply this embedding and quenched averaging framework to ternary, quaternary, and quinary alloys on fcc and bcc host lattices and discuss the numerical results in turn.

A. Ergodic identification of ensemble- and trajectory-averaged drag

Before proceeding, we must mention that the computation in Sec. VI treats the dislocation as static inside a random inner region and forms an ensemble average over disorder realizations. Mesoscale dynamics, however, concerns a moving line whose core neighborhood changes along its glide trajectory. It is nonobvious whether both viewpoints are equivalent; here we show that they are as an ergodic limit. Indeed, the equality of these two viewpoints is an ergodic statement, once the sequence of environments encountered by the core is modeled as a stationary ergodic process under translations along the glide direction.

We formalize this as follows: Let $(\Omega, \mathcal{F}, \mathbb{P})$ carry an environment field η defined on $\mathbb{R}$ (or $\mathbb{Z}$), equipped with a measure preserving translation action $(\tau_x)_{x \in \mathbb{R}}$ such that $\eta(x) = \eta(0) \circ \tau_x$ and such that the action is ergodic. The object $\eta(x)$ is an abstract encoding of the local chemistry and harmonic data seen by the core at glide position x , for instance, the restriction of the force constant field (and any auxiliary core descriptors used in the Kanzaki construction) to a fixed neighborhood of the glide plane, expressed in a comoving frame.

For each lag $\theta \geq 0$ we assume that the conditional mobility kernel at lag θ is a measurable functional of the environment at the earlier time, in the sense that there exists a measurable map

$$G_\theta: \Omega \rightarrow \mathbb{R} \quad (87)$$

such that, for a dislocation whose core is at position $X(t_0)$ at time t_0 , the kernel entering the linear mobility law at lag θ is

$$\Gamma_{\eta(X(t_0))}(\theta) = G_\theta(\tau_{X(t_0)}\eta(0)). \quad (88)$$

We further assume integrability at fixed lag,

$$G_\theta \in L^1(\mathbb{P}) \quad \text{for every } \theta \geq 0, \quad (89)$$

and, when Laplace space statements are needed, the joint integrability condition

$$\int_0^\infty \mathbb{E}_{\mathbb{P}}[|G_\theta|]d\theta < \infty. \quad (90)$$

The ensemble-averaged kernel is then

$$\bar{\Gamma}(\theta) = \mathbb{E}_{\mathbb{P}}[G_\theta]. \quad (91)$$

To connect with a moving dislocation, consider first a constant velocity trajectory $X(t) = vt$ with $v \neq 0$. Define the trajectory average of the lag kernel by

$$\Gamma_T(\theta) = \frac{1}{T} \int_0^T G_\theta(\tau_{vt}\eta(0))dt. \quad (92)$$

Since (τ_x) is ergodic and measure preserving, the induced flow $t \mapsto \tau_{vt}$ is ergodic and measure preserving as well. Birkhoff's ergodic theorem [107] for flows therefore yields the almost sure limit, for each fixed $\theta \geq 0$,

$$\lim_{T \rightarrow \infty} \Gamma_T(\theta) = \bar{\Gamma}(\theta), \quad \mathbb{P} \text{ almost surely.} \quad (93)$$

A discrete sampling version, relevant when the dislocation traverses environments in increments $\Delta X \neq 0$, is obtained by applying Birkhoff's theorem to the transformation $S = \tau_{\Delta X}$:

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} G_\theta(\tau_{n\Delta X}\eta(0)) = \bar{\Gamma}(\theta), \quad \mathbb{P} \text{ almost surely.} \quad (94)$$

This identifies the configuration average used in Sec. VI with the long-time average sampled by a single dislocation moving through the statistically stationary alloy, conditional on the modeling assumption Eq. (88).

Under the integrability condition Eq. (90), dominated convergence upgrades pointwise convergence Eq. (93) to convergence of Laplace transforms. Writing $\hat{\Gamma}_T(s) = \int_0^\infty e^{-s\theta} \Gamma_T(\theta) d\theta$ for $\text{Re } s > 0$, one has

$$\lim_{T \rightarrow \infty} \hat{\Gamma}_T(s) = \hat{\bar{\Gamma}}(s), \quad \hat{\bar{\Gamma}}(s) \equiv \int_0^\infty e^{-s\theta} \bar{\Gamma}(\theta) d\theta, \quad (95)$$

In particular, the imaginary axis evaluations used in Stieltjes fitting are interpreted as boundary values of $\hat{\bar{\Gamma}}(s)$, and the static drag obtained from $\hat{\bar{\Gamma}}(0)$ is, in the above sense, the almost sure long-time average of the drag experienced by a single line.

The constant velocity assumption is the natural setting for the strict ergodic identification because it converts spatial stationarity into a measure preserving temporal flow. For general monotone trajectories, one may still obtain an ergodic identification by reparametrizing time by arc length, or by imposing additional mixing hypotheses that control the time change induced by $X(t)$; since the mesoscale mobility law is used primarily in regimes in which the velocity varies slowly compared with the kernel support, the constant velocity identification above suffices.

B. Bookkeeping: Single-line normalization, diagnostics, and averaging order

The embedded dipole calculation returns, for each configuration $\mathcal{C}$, a 2×2 causal kernel matrix $\hat{\Gamma}_{ij}^{(\mathcal{C})}(s)$ relating the two Peach–Koehler forces F_i to the two velocities v_j via $\hat{F}_i(s) = \sum_j \hat{\Gamma}_{ij}^{(\mathcal{C})}(s) \hat{v}_j(s)$, with $i, j \in \{1, 2\}$. Mesoscale mobility laws require a per-line kernel. Throughout this section, we therefore define the per-line self kernel before any low-frequency limiting procedure by

$$\hat{\Gamma}_{\text{self}}^{(\mathcal{C})}(s) = \frac{1}{2} (\hat{\Gamma}_{11}^{(\mathcal{C})}(s) + \hat{\Gamma}_{22}^{(\mathcal{C})}(s)), \quad \bar{\hat{\Gamma}}(s) = \langle \hat{\Gamma}_{\text{self}}^{(\mathcal{C})}(s) \rangle_{\mathcal{C}}, \quad (96)$$

and we set

$$B = \bar{\hat{\Gamma}}(0). \quad (97)$$

The same normalization is used at finite temperature, because thermal occupation enters multiplicatively through Bose factors in the mode sums and therefore preserves the linear decomposition implicit in Eq. (96) at the level of the matrix elements.

Two numerical diagnostics extracted from the dipole data quantify whether the single-line extraction is uncontaminated by coherent cross-dissipation and whether the sampling is symmetric. Let $B_{C,ab}^{(1)} = \hat{\Gamma}_{C,ab}^{(1)}(0)$ be the configuration-resolved static matrix elements and let B_{11} , B_{22} , B_{12} denote their disorder averages after conversion to the same per line normalization as in Eq. (97). Exchangeability of the two core positions implies $\langle B_{C,11}^{(1)} \rangle_{\mathcal{C}} = \langle B_{C,22}^{(1)} \rangle_{\mathcal{C}}$, so deviations quantify residual asymmetry in the sampling protocol. The coherence ratio

$$r = \frac{B_{12}}{\sqrt{B_{11}B_{22}}}, \quad (98)$$

satisfies $|r| \leq 1$ by Cauchy–Schwarz and is expected to obey $|r| \ll 1$ when the dipole separation is large compared with the disorder coherence length at the frequencies dominating the kernel. The equipartitioned estimate $B_{\text{equip}} = \frac{1}{2}(B_{11} + B_{22})$ provides a direct self-term estimate, and its agreement with the opposite sign projection estimate from Eq. (66) is a practical check that r is small.

Finally, the order of averaging and reduction matters. The class of Stieltjes functions is closed under convex averaging of the functions themselves, hence one must average the kernels (or, equivalently, their spectral measures) first and fit a Stieltjes surrogate only afterward. Averaging fitted pole parameters does not, in general, preserve the Stieltjes structure and therefore does not preserve passivity or complete monotonicity.

C. Numerical results

We apply the embedding and quenched averaging formalism to ternary, quaternary, and quinary alloys on face-centered cubic and body-centered cubic host lattices. Interatomic interactions are described by the embedded-atom method (EAM) or MLIP, depending on the system, with all force constants extracted from fully relaxed supercells, as described in Sec. VI. For each composition, between 10 and 20 independent chemical configurations are generated using SQS structures. For each configuration $\mathcal{C}$, we compute the configuration-resolved kernel $\hat{\Gamma}^{(\mathcal{C})}(i\xi)$ on a logarithmically

TABLE I. Ensemble-averaged drag and two-pole Stieltjes fit parameters for the ensemble-averaged memory kernel $\bar{\Gamma}(i\xi)$. Uncertainties are one standard deviation across configurations. The factor $r = B_{12}/\sqrt{B_{11}B_{22}}$ is the coherence ratio. Results are shown at zero thermal occupation to establish a baseline. B_{eff} represents the drag coefficient computed in the equivalent VCA effective medium. The following potentials were employed: for systems AlWMo, AlWMoTi, AlWMoTiFe with the EAM potential [108]; for FeCoNiCuCr with the EAM potential [109]; for AlMoWCrTi with the MLIP [110]. Drag is reported per unit dislocation line.

Composition	Character	T (K)	$B = \bar{\Gamma}(0)$ ($\mu\text{Pa s}$)	B_{eff} ($\mu\text{Pa s}$)	τ_1 (ps)	w_1 ($\mu\text{Pa s}$)	τ_2 (ps)	w_2 ($\mu\text{Pa s}$)	r
Al _{0.5} W _{0.25} Mo _{0.25}	$\langle 110 \rangle \{111\}$ screw	0	3.30 (0.36)	0.76	0.76	1.47	0.18	1.83	0.103 (0.022)
	$\langle 110 \rangle \{111\}$ edge	0	2.03 (0.16)	0.39	0.82	0.75	0.19	1.29	0.084 (0.021)
Al _{0.25} W _{0.25} Mo _{0.50}	$\langle 110 \rangle \{111\}$ screw	0	6.80 (2.80)	1.48	0.52	2.33	0.14	4.48	0.104 (0.027)
	$\langle 110 \rangle \{111\}$ edge	0	3.79 (1.61)	1.27	0.39	1.28	0.14	2.52	0.093 (0.022)
Al _{0.25} W _{0.5} Mo _{0.25}	$\langle 110 \rangle \{111\}$ screw	0	4.71 (0.54)	1.22	0.69	0.99	0.23	3.72	0.105 (0.024)
	$\langle 110 \rangle \{111\}$ edge	0	2.13 (0.16)	0.96	0.58	0.57	0.24	1.57	0.045 (0.14)
Al _{0.33} W _{0.33} Mo _{0.33}	$\langle 110 \rangle \{111\}$ screw	0	4.17 (0.34)	2.23	0.71	1.42	0.19	2.74	0.104 (0.022)
	$\langle 110 \rangle \{111\}$ edge	0	1.93 (0.09)	1.25	0.48	0.40	0.16	1.53	0.097 (0.026)
Al _{0.33} W _{0.33} Mo _{0.33} (MLIP)	$\langle 110 \rangle \{111\}$ screw	0	11.76 (0.21)	3.93	0.88	6.37	0.17	5.38	0.124 (0.010)
	$\langle 110 \rangle \{111\}$ edge	0	7.91 (0.42)	1.04	0.73	3.41	0.16	4.49	0.102 (0.032)
Al _{0.33} Ti _{0.33} Mo _{0.33}	$\langle 110 \rangle \{111\}$ screw	0	2.77 (0.29)	2.62	0.63	0.78	0.20	1.99	0.100 (0.032)
	$\langle 110 \rangle \{111\}$ edge	0	1.56 (0.11)	1.35	0.60	0.22	0.24	1.34	0.069 (0.035)
Al _{0.25} Ti _{0.25} W _{0.25} Mo _{0.25}	$\langle 110 \rangle \{111\}$ screw	0	3.31 (0.23)	1.08	0.84	1.05	0.19	2.26	0.092 (0.026)
	$\langle 110 \rangle \{111\}$ edge	0	2.23 (0.32)	0.47	0.51	0.76	0.16	1.48	0.024 (0.017)
Al _{0.2} Ti _{0.2} W _{0.2} Mo _{0.2} Fe _{0.2}	$\langle 110 \rangle \{111\}$ screw	0	8.51 (4.01)	0.65	0.74	2.99	0.17	5.51	0.103 (0.026)
	$\langle 110 \rangle \{111\}$ edge	0	3.91 (1.64)	0.18	0.52	1.12	0.16	2.79	0.026 (0.014)
Al _{0.2} Mo _{0.2} W _{0.2} Cr _{0.2} Ti _{0.2} (MLIP)	$\langle 111 \rangle \{110\}$ screw	0	15.20 (0.49)	4.90	0.76	7.48	0.20	7.72	0.106 (0.018)
	$\langle 111 \rangle \{110\}$ edge	0	8.63 (1.34)	6.62	0.66	3.62	0.19	5.02	0.102 (0.012)
Fe _{0.33} Co _{0.33} Ni _{0.33}	$\langle 111 \rangle \{110\}$ screw	0	15.28 (0.04)	2.23	0.61	3.96	0.16	11.33	0.106 (0.002)
	$\langle 111 \rangle \{110\}$ edge	0	2.83 (0.03)	1.70	1.47	0.81	0.22	2.03	0.014 (0.003)
Fe _{0.25} Co _{0.25} Ni _{0.25} Cu _{0.25}	$\langle 111 \rangle \{110\}$ screw	0	14.46 (0.04)	0.77	0.67	3.88	0.17	10.58	0.107 (0.001)
	$\langle 111 \rangle \{110\}$ edge	0	2.77 (0.12)	0.20	1.63	0.84	0.24	1.93	0.012 (0.006)
Fe _{0.2} Co _{0.2} Ni _{0.2} Cu _{0.2} Cr _{0.2}	$\langle 111 \rangle \{110\}$ screw	0	14.55 (0.05)	1.81	0.77	3.65	0.18	10.91	0.096 (0.005)
	$\langle 111 \rangle \{110\}$ edge	0	2.88 (0.03)	0.44	1.67	1.00	0.24	1.88	0.024 (0.049)

spaced imaginary frequency grid and report quenched ensemble averages $\bar{\Gamma}(i\xi) = \langle \hat{\Gamma}^{(C)}(i\xi) \rangle_C$ together with uncertainties given by one standard deviation across configurations. Unless stated otherwise, all results in this section correspond to zero thermal occupation so as to isolate the quantum zero-point contribution to phonon-mediated dissipation; they can be found tabulated in Table I.

1. Kernel shape and reduced-order representation

Across all systems and dislocation characters considered, the disorder-averaged imaginary axis kernel $\bar{\Gamma}(i\xi)$ is smooth, positive, and monotonically decreasing in ξ , approaching a finite static limit $B = \bar{\Gamma}(0)$ as $\xi \rightarrow 0$. Over the resolved low-frequency band, $\bar{\Gamma}(i\xi)$ remains close to its static plateau and then crosses over into a gradual decay across the vibrational bandwidth. This confirms that, on sufficiently long timescales, the mobility law admits an effectively Markovian reduction, with non-Markovian corrections confined to the regime in which the defect dynamics probes frequencies for which $\bar{\Gamma}(i\xi)$ departs appreciably from B .

To quantify the onset of frequency dependence without assigning a microscopic meaning to any single crossover point, we define an operational crossover frequency ξ_ε by

$|\bar{\Gamma}(i\xi_\varepsilon) - B|/B = \varepsilon$, with fixed ε , and the associated timescale $\tau_\varepsilon = \xi_\varepsilon^{-1}$. When the spectral content of the defect velocity is concentrated at $\xi \ll \xi_\varepsilon$, the replacement $\bar{\Gamma}(i\xi) \mapsto B$ incurs only an $O(\varepsilon)$ relative error in the friction law, whereas motion that samples $\xi \gtrsim \xi_\varepsilon$ necessarily probes the hereditary character of the kernel.

For stable time integration and reduced-order modeling, we approximate $\bar{\Gamma}(i\xi)$ by the rational Stieltjes surrogate in Eq. (109). In practice, one or two poles suffice to reproduce the kernel shape over the fitted band for all cases examined. Increasing the order beyond two does not expose additional robust structure on the resolved window and instead produces near degeneracies in the fitted nodes under the positivity and moment constraints. In line with the interpretation in Sec. VIH, the parameters (w_m, Ω_m) should therefore be regarded as effective quadrature data for a structure preserving surrogate, while the robust observables reported by the calculation remain the static drag B together with the band-limited shape of $\bar{\Gamma}(i\xi)$.

Figures 3 and 4 illustrate the two-pole surrogate for representative screw dislocations in equiatomic bcc AlWMoTiFe and equiatomic fcc FeCoNiCuCr, chosen to span the range of drag magnitudes in Table I. In both systems, the surrogate reproduces the static plateau and the subsequent crossover

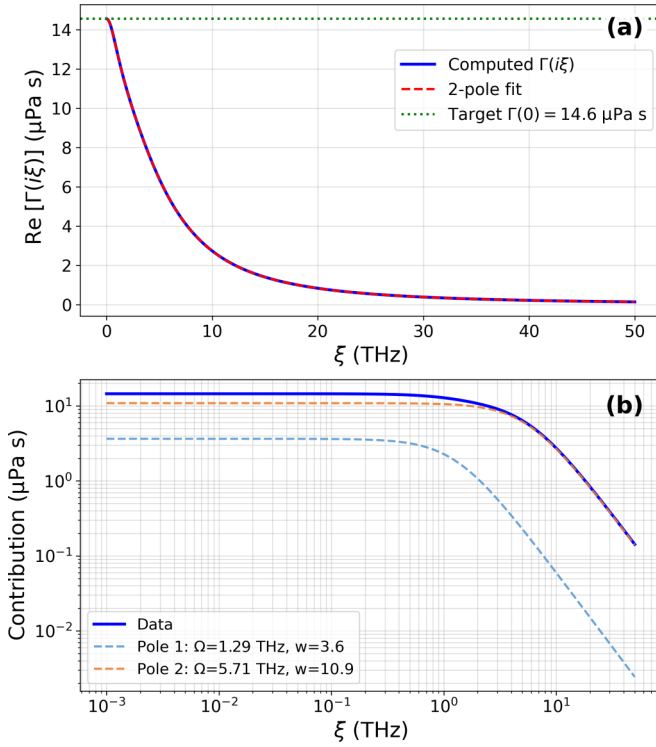


FIG. 3. (a) Disorder-averaged imaginary axis kernel $\bar{\Gamma}(i\xi)$ and two-pole Stieltjes fit for the screw dislocation dipole in the embedded region, in equiatomic fcc FeCuCoNiCr at zero thermal occupation. Panel (b) shows the corresponding pole contributions.

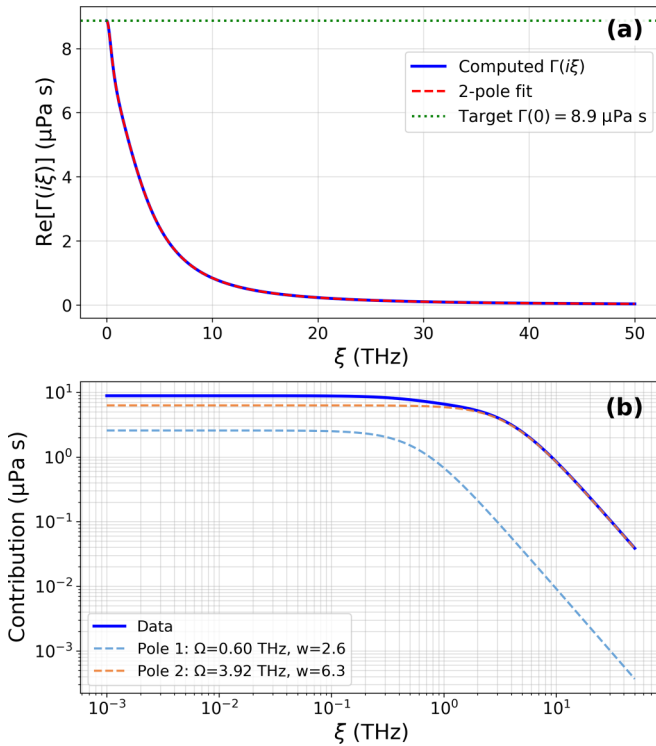


FIG. 4. (a) Disorder-averaged imaginary axis kernel $\bar{\Gamma}(i\xi)$ and two-pole Stieltjes fit for the screw dislocation dipole in the embedded region in equiatomic bcc AlWMoTiFe at zero thermal occupation. Panel (b) shows the corresponding pole contributions.

TABLE II. Elemental reference static drags at zero thermal occupation, computed using the same embedding protocol as in Table I, but in an ordered system. Values are for edge and screw character, per unit dislocation line.

Element	Lattice	B_{edge} ($\mu\text{Pa s}$)	B_{screw} ($\mu\text{Pa s}$)
Al	fcc	1.10	6.57
Ni	fcc	2.43	15.18
Cu	fcc	2.05	12.94
W	bcc	5.33	6.59
Fe	bcc	2.43	2.76
Mo	bcc	2.79	4.34

into decay across the entire fitted band. The fitted nodes are consistently of order a few terahertz, corresponding to subpicosecond timescales, and the weights partition B in a manner that reflects the material and character dependence. Within the present bandwidth, no additional stable pole structure is required beyond this minimal representation; all other results reported in Table I exhibit an analogous structure.

As a validation of the per-line drag scale, we applied the same line-projected spectral construction to ordered elemental crystals, where comparison with published dislocation mobility data are meaningful. The coefficients in Table II are line drag coefficients defined by the force balance $b\tau = Bv$ and should therefore be compared with atomistic mobility coefficients reported in units of Pa s , rather than with macroscopic viscosities. Starting from the $T \rightarrow 0$ baselines of Eq. (104) and using the calculated spectral slopes to extrapolate to room temperature, we obtain $B \simeq 6$ (edge) and 36 $\mu\text{Pa s}$ (screw) for Al, 11 and 69 $\mu\text{Pa s}$ for Ni, and 127 and 147 $\mu\text{Pa s}$ for W. These values are of the same per-line mobility scale as published phonon drag and atomistic mobility data: fcc Al and Ni values of $B_{\text{edge}} = 11.4 \pm 0.3$ and $B_{\text{screw}} = 20.3 \pm 2.3$ $\mu\text{Pa s}$ for Al, and $B_{\text{edge}} = 15.5 \pm 0.5$ and $B_{\text{screw}} = 18.0 \pm 1.4$ $\mu\text{Pa s}$ for Ni [17], comparable values for Cu from first-principles phonon wind calculations, with $B_{\text{edge}} \approx 24$ and $B_{\text{screw}} \approx 31$ $\mu\text{Pa s}$ [15], edge and screw coefficients of order 45 – 170 and 240 – 290 $\mu\text{Pa s}$ for $\frac{1}{2}\langle 111 \rangle\{110\}$ dislocations in α -Fe [18,111], and several hundred $\mu\text{Pa s}$ for W [112]. Pointwise numerical agreement should not be expected, principally because the present calculations use broad, transferable interatomic force fields (see Ref. [108] for Al, W, Mo and Ref. [109] for Ni, Fe) intended for multicomponent alloy calculations, whereas the reference MD studies generally use element-specific potentials optimized for the corresponding pure crystal and its defect properties. Additional differences arise from the fitting protocol followed to extract the drag coefficient from stress-velocity trajectories [17], the dislocation character and slip geometry [18,111], core spreading or dissociation [113], temperature [17,111], velocity window, finite size, and boundary effects, and the thermostatting and load-application protocol [18]. The relevant validation is therefore that the ordered limit reproduces the correct per line drag scale and the correct screw vs edge spread, and, whenever available, similar thermal slopes; the subsequent alloy calculations then quantify how configurational disorder reshapes that same line mobility quantity.

2. Static drags, character hierarchy, and Leibfried's law

Table I summarizes the ensemble-averaged static drags $B = \bar{\Gamma}(0)$ together with the two-pole Stieltjes parameters of the averaged kernels. Two clear trends emerge. First, screw dislocations consistently exhibit larger drag than edge dislocations at the same composition, and the magnitude of B varies strongly with composition within each character. We also note that the coherence ratio $r = B_{12}/\sqrt{B_{11}B_{22}}$ on the table results has been kept small across all systems, typically of order 10^{-2} to 10^{-1} , by choosing a sufficiently large supercell that ensures in each case that cross-dissipation be subdominant, and that the equipartitioned drag $B_{\text{equip}} = \frac{1}{2}(B_{11} + B_{22})$ accurately approximates the single-line drag, thereby validating the dipole embedding as a practical route to mobility parameters in chemically disordered alloys.

The systematic hierarchy $B_{\text{screw}} > B_{\text{edge}}$ follows directly from the structure of the quadratic dissipation functional. In our formulation,

$$B \propto \sum_v \frac{|\langle e_v, g \rangle|^2}{\omega_v^2} [2n_B(\omega_v) + 1], \quad (99)$$

where $g = \partial_X f^K$ is the driving field obtained by differentiating the Kanzaki force distribution with respect to dislocation position, and (e_v, ω_v) are eigenmodes of the embedded lattice. The distinction between screw and edge character enters entirely through the geometry of g . A screw dislocation carries a pure shear Volterra field, with displacement parallel to the line and a stress field that is entirely deviatoric, whereas an edge dislocation has mixed shear and dilatational character and hence a nonzero hydrostatic component. This distinction enters Eq. (99) only through the geometry of the Kanzaki driving field $g = \partial_X f^K$: the screw driving field is dominated by shear components and therefore projects efficiently onto transverse phonon eigenvectors, while the edge driving field has a comparatively larger longitudinal projection associated with its dilatational part. Since the ω_v^{-2} weighting emphasizes low-frequency modes for which transverse branches dominate the response, the net projected spectral weight is generically larger for screw character, yielding $B_{\text{screw}} > B_{\text{edge}}$.

Quantitatively, the screw to edge ratio spans approximately 1.63 to 2.21 across the Al–Mo–W ternary compositions reported, varying between about 1.48 in the AlTiWMo and 2.18 in AlTiWMoFe, and is larger still in the fcc Fe based systems: for $\text{Fe}_{0.33}\text{Co}_{0.33}\text{Ni}_{0.33}$ we obtain $B_{\text{screw}}/B_{\text{edge}} \simeq 5.4$, for $\text{Fe}_{0.25}\text{Co}_{0.25}\text{Ni}_{0.25}\text{Cu}_{0.25}$ the ratio is approximately 5.2, yet for $\text{Fe}_{0.2}\text{Co}_{0.2}\text{Ni}_{0.2}\text{Cu}_{0.2}\text{Cr}_{0.2}$ it is approximately 5.1. Within a fixed character, the compositional dependence is substantial. For screw dislocations in the Al–Mo–W ternary, B ranges from 3.30 $\mu\text{Pa s}$ in $\text{Al}_{0.5}\text{W}_{0.25}\text{Mo}_{0.25}$ to 6.80 $\mu\text{Pa s}$ in $\text{Al}_{0.25}\text{W}_{0.25}\text{Mo}_{0.5}$, while edge drags span 1.93 $\mu\text{Pa s}$ to 3.79 $\mu\text{Pa s}$. In the fcc quinary $\text{Fe}_{0.2}\text{Co}_{0.2}\text{Ni}_{0.2}\text{Cu}_{0.2}\text{Cr}_{0.2}$ the screw drag reaches 14.55 $\mu\text{Pa s}$, about two to four times larger than the Al–Mo–W ternary screws, indicating that chemical complexity reshapes the projected spectral measure rather than merely rescaling bulk elastic descriptors. We leave the discussion of MLIP data to Sec. VII C 6.

Phonon drag in HEAs and Leibfried's law. It is instructive to contrast these results with the classical Leibfried phonon wind picture [81], not as an external benchmark but as the con-

tinuum expectation one would reach by suppressing precisely the ingredients retained here. According to Leibfried's law, in its standard regime, a dislocation moving at low velocity in a fixed crystalline host experiences a viscous drag whose dominant temperature contribution is approximately linear in T , with the prefactor expressed in terms of bulk elastic and vibrational descriptors of that host, namely:

$$B \propto \gamma^2 k_B \frac{T}{c^2},$$

with c the host lattice's speed of sound, and γ its Grüneisen parameter. In this picture, upon alloying a metal, the only changes to the phonon drag would arise from modifications that alloying may make to the effective elastic constants, density, and anharmonicity of the lattice. Given that alloying, at least in a dilute setting, is expected to increase c and γ , it has been argued in the context of dilute alloying (e.g., Refs. [17, 114]) that phonon drag ought to be expected to increase as the system is alloyed.

This may very well be reasonable, but the results in Table I are incompatible with this picture in a way that is not merely quantitative but structural. Leibfried's derivation evaluates phonon dislocation scattering *qua* plane-wave phonon states of definite wave vector and polarization, each residing on a sharp dispersion branch. In a concentrated alloy, however, both mass- and force-constant-disorder broaden the vibrational spectral functions and fragment the line-projected Fourier content of the modes. Once the disorder-induced linewidth becomes comparable with the mode frequency, which is precisely the regime approached by short wavelength branches in the systems studied here, the kinematic picture underlying a single event between well-defined initial and final phonon states is no longer controlled. The relevant object is then not a rate constructed from delta functions on sharp dispersions, but an embedded spectral measure that already incorporates disorder-induced broadening and localization through the resolvent.

The same structural issue arises in the treatment of the coupling. Leibfried's continuum picture assumes a translationally invariant interaction vertex, so that a single Grüneisen parameter γ may be taken to encode the anharmonicity relevant for drag. In a chemically disordered lattice, by contrast, the Kanzaki vertex is intrinsically configuration dependent: the mode-resolved coupling $g_{\nu c}$ fluctuates with the local chemical environment sampled by the core and its near field. Since dissipation is quadratic in the coupling, the configurational average enters as $\langle |g_{\nu c}|^2 \rangle_c$ rather than $|\langle g_{\nu c} \rangle_c|^2$, with the variance contribution $\langle |g|^2 \rangle - |\langle g \rangle|^2 \geq 0$ representing an irreducible enhancement absent from any homogenized, host parameter description. This distinction is immaterial in an ordered crystal, but it becomes leading order in a concentrated alloy precisely because the disorder that broadens the phonon spectrum also amplifies fluctuations in the dislocation phonon coupling near the core.

Finally, the Leibfried picture assumes a Markovian reduction in which the bath correlation time is short compared with the timescale of defect motion, so that drag is represented by a single, velocity-independent coefficient B . In the present formulation the natural outcome of integrating out the lattice is instead a retarded mobility kernel, and in a disordered alloy

the broadened and fragmented spectral landscape generically produces a nontrivial frequency dependence of the disorder-averaged response $\bar{\Gamma}(\omega)$. The low-frequency limit $\bar{\Gamma}(0)$ is then not required to coincide with what one would obtain by inserting averaged elastic constants into a host-based scaling law, because it is the value remaining after the full relaxation structure encoded in $\bar{\Gamma}(\omega)$ has been resolved. The emergence of a stable Stieltjes pole representation, as reported in Table I, is therefore not a fitting convenience but a direct signature that the Markovian contraction of the lattice response is itself a nontrivial step whose validity must be assessed rather than assumed.

The data in Tables I and II provide a direct test of what can and cannot be inferred from a host-based phonon wind picture. Leibfried's law predicts the thermal scaling of drag within a fixed crystalline host in terms of bulk descriptors such as the sound speed and Grüneisen parameter. What is nontrivial in a concentrated multicomponent alloy is whether the magnitude of the drag can be inferred from composition by treating the alloy as an effectively homogeneous host.

The fcc systems are particularly instructive. For the ternary $\text{Fe}_{0.33}\text{Co}_{0.33}\text{Ni}_{0.33}$ we obtain an edge drag of $2.83 \mu\text{Pa s}$, essentially coincident with elemental Ni at $2.43 \mu\text{Pa s}$ (Table II). The quaternary $\text{Fe}_{0.25}\text{Co}_{0.25}\text{Ni}_{0.25}\text{Cu}_{0.25}$ yields $2.77 \mu\text{Pa s}$, slightly below the Ni reference and only modestly below elemental Cu at $2.05 \mu\text{Pa s}$. In neither case does alloying elevate significantly the drag beyond the scale already set by the largest elemental constituent. By contrast, the quinary $\text{Fe}_{0.2}\text{Co}_{0.2}\text{Ni}_{0.2}\text{Cu}_{0.2}\text{Cr}_{0.2}$ gives $2.88 \mu\text{Pa s}$, exceeding both Ni and Cu and approaching the elemental Cr reference of $1.971 \mu\text{Pa s}$, despite the nearly identical masses of the constituent elements. In neither case does alloying elevate the drag beyond the scale already set by the largest elemental constituent. By contrast, the quinary gives a value exceeding both Ni and Cu. The effect of alloying is therefore not monotone: increasing chemical complexity may suppress or enhance drag relative to elemental values, and cannot be inferred from a simple interpolation of bulk descriptors.

A similar conclusion follows in the bcc refractory family. The Al–W–Mo ternary edge drags span $1.93\text{--}3.79 \mu\text{Pa s}$, below elemental W at $5.33 \mu\text{Pa s}$ and about the same as Fe at $2.43 \mu\text{Pa s}$, even for tungsten fractions as high as 50%. Alloy drag is therefore neither bounded above by the stiffest constituent nor determined by a composition weighted average of elemental drags. The addition of further elements may either increase or decrease the drag, depending on how local mass and force constant fluctuations reshape the projected spectral measure entering Eq. (99).

Whereas for the reasons stated above Leibfried's law cannot account for phonon drag trends in heavily disordered systems, in the present formulation this behavior has a natural explanation, rooted on the same interpretation as that offered for the failure of effective medium theories (see Sec. VIC). Indeed, the static drag is a quadratic functional of the configuration-dependent Kanzaki coupling, weighted by the embedded spectral measure. Composition acts not only by modifying averaged elastic constants, but by altering both the statistics of the coupling and the distribution of spectral weight in frequency space. Because the drag depends on $\langle |g|^2 \rangle_c$ rather than $| \langle g \rangle_c |^2$, fluctuations in

local chemistry enter at leading order. Depending on whether additional species increase or decrease the variance of the projected coupling to low-frequency modes, alloying may enhance or suppress the drag. This mechanism is invisible in any description that retains only homogenized host parameters.

Taken together, these results show that while Leibfried's phonon wind scaling remains internally consistent within its regime of application, it does not constitute a predictive closure on composition for concentrated HEAs. In particular, the assumption that increasing chemical complexity necessarily enhances phonon drag and, by extension, dynamic dissipation is not supported by the present calculations nor by the physics of phonon drag; design strategies that rely on such monotonicity may therefore optimize toward compositions whose actual drag response is controlled by variance effects invisible to the guiding model. Our embedding and configurational averaging framework replaces this kind of extrapolation by a direct evaluation of the disorder-averaged spectral measure and its associated mobility kernel, yielding quantitative drag coefficients and, when required, compact pole representations suitable for time domain mobility laws.

3. Effective medium failure and the role of variance

One of the central theoretical results of this work is that effective medium constructions underestimate dislocation drag because they average too early. Indeed, across all systems in Table I, the effective medium (virtual crystal) drag, computed by placing the same system on an effective medium rather than an atomistically disordered supercell, is not a mild underestimate of the disorder-averaged value but is suppressed to the point that it often lies below the range spanned by the elemental constituents (Table II), and generally one or two orders of magnitudes below the fully atomistic drag averages we report in Table I.

The magnitude of the effective medium suppression can be illustrated concretely by two representative cases. For the equiatomic bcc Al–W–Mo alloy, the disorder-averaged drag is $\bar{B}_{\text{screw}} = 4.17 \mu\text{Pa s}$ and $\bar{B}_{\text{edge}} = 1.93 \mu\text{Pa s}$, whereas the corresponding virtual crystal values are $B_{\text{screw}}^{\text{eff}} = 2.23 \mu\text{Pa s}$ and $B_{\text{edge}}^{\text{eff}} = 1.25 \mu\text{Pa s}$. The effective medium therefore underestimates the screw drag by a factor of 1.9 and the edge drag by a factor of 1.5, and collapses the screw-to-edge ratio from 2.16 to 1.78, eliminating the strong character contrast. An even more extreme suppression occurs in the fcc FeCoNi system, where $\bar{B}_{\text{screw}} = 15.28 \mu\text{Pa s}$ and $\bar{B}_{\text{edge}} = 2.83 \mu\text{Pa s}$, while the virtual crystal yields $B_{\text{screw}}^{\text{eff}} = 2.23 \mu\text{Pa s}$ and $B_{\text{edge}}^{\text{eff}} = 0.17 \mu\text{Pa s}$. Here, the effective medium underestimates the drag by factors of 6.9 and 16.6, respectively, and reduces the screw-to-edge ratio from 5.4 to 13.1.

This behavior can be understood by examining what the effective medium approximation does at the level of the objects entering the drag functional. In a real elemental crystal, the Kanzaki coupling g and the phonon spectrum are generated by the same force constant matrix Φ , so that the magnitude of the coupling and the distribution of spectral weight are intrinsically correlated. The VCA breaks this correlation by independently averaging masses and force constants to construct a fictitious translationally invariant lattice. Since the drag coefficient is quadratic in the coupling, this independent

averaging replaces $\langle |g|^2 \rangle_C$ by $|\langle g \rangle_C|^2$ and thereby removes all variance contributions associated with local chemical environments.

We also note that more sophisticated effective medium theories have been developed for disordered phonons beyond single-site VCA or CPA. Cluster extensions, including phonon dynamical cluster approaches and typical medium variants, retain nonlocal disorder correlations and can describe disorder-induced phonon localization through typical rather than only arithmetic spectral functions [55,56,58]. These methods provide systematic improvements for the bulk disordered vibrational problem, especially when mass and force constant disorder produce strong spectral broadening or localization. Their scope is nevertheless distinct from the obstruction identified here. The drag kernel is a quadratic functional of the configuration-dependent Kanzaki source and of the retarded response projected onto the dislocation core region. A homogeneous effective medium, even when cluster improved, does not by itself retain the variance contribution associated with the local chemical environments sampled by the core unless the source and inner Green's function are kept configuration-resolved before averaging. Cluster effective media could therefore be used as improved far-field baths within the present embedding construction, but they do not remove the need for an explicitly resolved disordered core region in the calculation of phonon drag.

In the bcc refractory systems, this suppression admits a particularly transparent scaling interpretation. At zero thermal occupation, the drag scales schematically as $B \sim |g|^2/\omega^2$. Since g scales with the local force constants Φ while $\omega^2 \sim \Phi/m$, a crude dimensional estimate gives $B \sim \Phi m$. When mass and stiffness are positively correlated across the constituent elements, as they are in the Al–W–Mo family where aluminum is both light and soft while tungsten and molybdenum are heavy and stiff, one has the covariance inequality $\langle \Phi \rangle \langle m \rangle \leq \langle \Phi m \rangle$. The virtual crystal computes the left-hand side, whereas the composition-weighted elemental average samples the right-hand side. The effective medium drag is therefore depressed below even the weakest elemental value by construction, without invoking any additional physics. The large separation between the VCA values and both the elemental and disorder-averaged drags in the bcc refractory alloys is a direct manifestation of this mass-stiffness covariance.

This argument, however, cannot account for the equally strong suppression observed in the fcc Fe-based systems, where the constituent masses are nearly identical and the covariance mechanism is absent. In that case, the failure of the effective medium has a different origin. The VCA force constants are averages over elements that do not share a common stable crystal structure: fcc iron is mechanically unstable at zero temperature, cobalt is hcp, and nickel alone stabilizes the fcc lattice. Averaging their force constants produces a fictitious dynamical matrix that is not realized by any actual crystal and whose phonon eigenvectors need not be geometrically aligned with the Kanzaki coupling generated by the averaged slip field. The resulting mismatch between the coupling geometry and the low-frequency spectral weight suppresses the drag even in the absence of strong mass fluctuations. In this sense, the effective medium does not merely

smooth disorder; it constructs a lattice whose dislocation-phonon coupling lacks the internal consistency present in any real constituent phase.

Taken together, these two mechanisms explain why the effective medium drag is not only quantitatively inaccurate but qualitatively misleading in concentrated alloys. In systems with strong mass-stiffness correlations, it suppresses drag through covariance effects, while in systems composed of elements from incompatible structural families, it produces a fictitious host whose coupling to lattice vibrations is intrinsically weak. In both cases, the virtual crystal approximation removes precisely the local chemical fluctuations that dominate the quadratic coupling functional controlling phonon-mediated dissipation.

Effective media and quadratic couplings. It bears pointing out that this suppression mechanism has implications beyond phonon drag. Indeed, any observable that depends quadratically on configuration-dependent couplings will exhibit an analogous enhancement under disorder averaging. To see this, let $\mathcal{O}^{(C)}$ be an observable computed for configuration C that takes the quadratic form

$$\mathcal{O}^{(C)} = \sum_v |\langle \phi_v, h^{(C)} \rangle|^2 W_v^{(C)}, \quad W_v^{(C)} \geq 0, \quad (100)$$

where $h^{(C)}$ is a configuration-dependent source or coupling field, $\{\phi_v\}$ is a complete basis, and $W_v^{(C)}$ are non-negative weights that may themselves depend on configuration. Energetic quantities generically assume this form: the elastic energy of a defect, the Peierls barrier for dislocation migration, the formation energy of a kink pair, and the stacking fault energy all involve quadratic functionals of displacement or strain fields that depend on the local chemical environment. Writing $h_v^{(C)} = \langle \phi_v, h^{(C)} \rangle$, apply Cauchy–Schwarz to the random variables $[W_v^{(C)}]^{1/2}$ and $[W_v^{(C)}]^{1/2} h_v^{(C)}$ to obtain, mode by mode,

$$|\langle W_v^{(C)} h_v^{(C)} \rangle_C|^2 \leq \langle W_v^{(C)} \rangle_C \langle W_v^{(C)} |h_v^{(C)}|^2 \rangle_C. \quad (101)$$

Rearranging and summing over v gives the lower bound

$$\begin{aligned} \langle \mathcal{O}^{(C)} \rangle_C &= \sum_v \langle W_v^{(C)} |h_v^{(C)}|^2 \rangle_C \\ &\geq \sum_v \langle W_v^{(C)} \rangle_C |\langle h_v^{(C)} \rangle_{C, W_v}|^2 \equiv \mathcal{O}^{(\text{eff})}, \end{aligned} \quad (102)$$

where $\langle \cdot \rangle_{C, W_v}$ denotes the $W_v^{(C)}$ weighted configurational average, $\langle h_v \rangle_{C, W_v} = \langle W_v^{(C)} h_v^{(C)} \rangle_C / \langle W_v^{(C)} \rangle_C$. Thus, for any quadratic observable with non-negative weights, any procedure that replaces the fluctuating couplings by an averaged coupling necessarily produces a lower bound on the disorder-averaged value. When the weights are configuration independent, $W_v^{(C)} \equiv W_v$, the lower bound sharpens to the identity

$$\langle \mathcal{O}^{(C)} \rangle_C = \sum_v W_v (|\langle h_v^{(C)} \rangle_C|^2 + \text{Var}_C(h_v^{(C)})) = \mathcal{O}^{(\text{eff})} + \Delta \mathcal{O}_{\text{var}}, \quad (103)$$

with $\Delta \mathcal{O}_{\text{var}} \geq 0$, which isolates the variance contribution discarded by an effective medium description. This is precisely the situation for phonon drag in the present harmonic framework, where the weights entering the Stieltjes representation

are fixed by the phonon spectrum and thermal occupations and are independent of the chemical realization; here, our calculations show that ΔB_{var} constitutes the dominant fraction of the total drag. Since the lower bound property holds in the general case and the variance identity makes its origin clear in the fixed weight case, we must conclude that whereas effective medium theories of disordered alloys provide a lower bound on any such quadratic observable, they cannot, in general, furnish an adequate estimate of its magnitude. This suggests that Peierls barriers, kink formation energies, and critical stresses computed from effective medium descriptions of disordered alloys may similarly underestimate the true disorder-averaged values, a point that merits systematic investigation.

4. Temperature dependence of dislocation drag

The zero thermal occupation values in Table I fix the $T \rightarrow 0$ limit of the Keldysh–Kanzaki influence functional, in which dissipation arises from spontaneous emission into the phonon bath. Within the present approximation, the retarded lattice response and the configuration-dependent Kanzaki vertex are temperature independent, being determined solely by the relaxed force constants and the embedded Green's function. Temperature enters through the symmetrized correlator, which supplies the universal factor $\coth(\beta\hbar\omega/2) = 2n_B(\omega) + 1$ in the mode-resolved spectral density. The entire thermal dependence is therefore a Bose reweighting of the same embedded spectral measure that fixes the zero-point contribution. For further details on the thermal dependency of this formulation, particularly at cryogenic temperatures, see Appendix C; here we focus on the full thermal occupation “high-temperature” regime, where phonon drag does not compete against electronic effects [82].

Writing the static drag in spectral form,

$$B(T) = \int_0^\infty \frac{d\omega}{\omega} \rho_0(\omega) \coth\left(\frac{\beta\hbar\omega}{2}\right), \quad (104)$$

with $\rho_0(\omega)$ the zero occupation spectral density produced by the embedding calculation, we separate a T -independent baseline by adding and subtracting unity,

$$B(T) = B_0 + \Delta B(T), \quad B_0 = \int_0^\infty \frac{d\omega}{\omega} \rho_0(\omega), \quad (105)$$

$$\begin{aligned} \Delta B(T) &= \int_0^\infty \frac{d\omega}{\omega} \rho_0(\omega) \left[\coth\left(\frac{\beta\hbar\omega}{2}\right) - 1 \right] \\ &= 2 \int_0^\infty \frac{d\omega}{\omega} \frac{\rho_0(\omega)}{e^{\beta\hbar\omega} - 1}. \end{aligned} \quad (106)$$

Equation (106) shows that thermal enhancement is controlled by the infrared part of ρ_0 : modes with $\hbar\omega \gg k_B T$ are exponentially suppressed, while modes with $\hbar\omega \lesssim k_B T$ contribute with classical occupation $n_B(\omega) \simeq k_B T / (\hbar\omega)$. Inserting this approximation into the thermally populated band yields the asymptotically linear law

$$B(T) \simeq B_0 + B' T, \quad B' = \frac{2k_B}{\hbar} \int_0^\infty \frac{d\omega}{\omega^2} \rho_0(\omega), \quad (107)$$

where the moment in Eq. (107) is finite in the present embedded construction because the effective medium subtraction

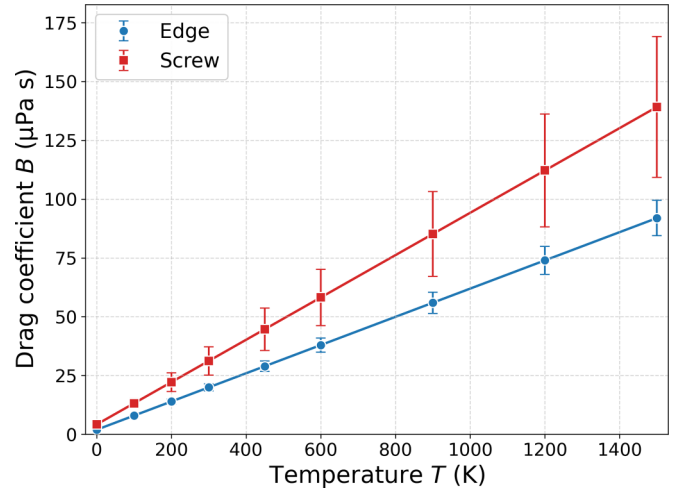


FIG. 5. Temperature dependence of the drag coefficients for edge and screw dislocations in the bcc AlWMo equimolar system. The linear fit to the averaged data were $B_{\text{edge}} = 0.21 + 0.058T$, $B_{\text{screw}} = 0.43 + 0.09T$ $\mu\text{Pa s}$, the fitting slopes showing excellent agreement with the thermal gradients predicted in Table III.

removes the long-wavelength elastic contribution discussed in Sec. VI C. The content of Eq. (107) is therefore not the trivial statement that B is linear in T , but that the thermal slope is a specific infrared-weighted spectral moment of the same ρ_0 that fixes B_0 . In practice, B' is dominated by the lowest part of the resolved spectrum because of the ω^{-2} kernel, whereas B_0 weights the spectrum only as ω^{-1} ; the thermal slope is thus a sharper probe of how disorder and composition reshape the line-projected coupling to long-wavelength acoustic modes.

Two averages appear naturally once one treats temperature and disorder at the same time. For each configuration, one may define the asymptotic thermal slope by the spectral moment

$$B'(C) = \frac{2k_B}{\hbar} \int_0^\infty \frac{\rho_0^{(C)}(\omega)}{\omega^2} d\omega, \quad (108)$$

and then form the quenched average $\bar{B}' = \langle B'(C) \rangle_C$. Alternatively, one may first average the full drag curve, $\bar{B}(T) = \langle B^{(C)}(T) \rangle_C$, and extract a slope by fitting $\bar{B}(T) \simeq \bar{B}_0 + (d\bar{B}/dT) T$ over the same temperature interval. Since $B^{(C)}(T)$ is a nonlinear functional of $\rho_0^{(C)}$, these two operations need not agree in principle. In the present calculations, however, they agree closely. For equiatomic AlWMo shown in Fig. 5, the slope inferred from the fit to $\bar{B}(T)$ is $0.05 \mu\text{Pa s K}^{-1}$ for edge and $0.09 \mu\text{Pa s K}^{-1}$ for screw, in near coincidence with $\bar{B}'$ obtained from Eq. (108). The small residual mismatch is confined to the low-temperature crossover near $T = 0$ and provides a useful consistency check that Bose reweighting and quenched averaging are being applied coherently: they should not match, because it is precisely at low temperatures that the linear thermal dependence breaks down.

The physical content of Eq. (107) is that B' is an infrared-weighted moment of the same projected spectral measure that fixes B_0 . Because B_0 weights ρ_0 by ω^{-1} while B' weights it by ω^{-2} , the thermal slope is a sharper probe of how composition and local chemistry reshape the coupling to long-wavelength

TABLE III. Thermal gradient $B' = dB/dT$ extracted from direct computation of the thermal slope [Eq. (107)] over 300–1500 K, averaged over 50 configurations. All results are reported per unit length.

Composition	Character	$B' (\mu\text{Pa s/K})$
$\text{Al}_{0.33}\text{Ti}_{0.33}\text{Mo}_{0.33}$	screw	0.06 ± 0.03
	edge	0.03 ± 0.01
$\text{Al}_{0.33}\text{W}_{0.33}\text{Mo}_{0.33}$	screw	0.09 ± 0.04
	edge	0.06 ± 0.01
$\text{Al}_{0.25}\text{W}_{0.25}\text{Mo}_{0.5}$	screw	0.16 ± 0.19
	edge	0.07 ± 0.11
$\text{Al}_{0.25}\text{W}_{0.5}\text{Mo}_{0.25}$	screw	0.10 ± 0.02
	edge	0.05 ± 0.01
$\text{Al}_{0.5}\text{W}_{0.25}\text{Mo}_{0.25}$	screw	0.09 ± 0.06
	edge	0.05 ± 0.03
$\text{Al}_{0.25}\text{W}_{0.25}\text{Mo}_{0.25}\text{Ti}_{0.25}$	screw	0.11 ± 0.09
	edge	0.04 ± 0.01
$\text{Al}_{0.2}\text{W}_{0.2}\text{Mo}_{0.2}\text{Ti}_{0.2}\text{Fe}_{0.2}$	screw	0.19 ± 0.23
	edge	0.08 ± 0.09
$\text{Fe}_{0.33}\text{Co}_{0.33}\text{Ni}_{0.33}$	screw	0.06 ± 0.01
	edge	0.03 ± 0.00
$\text{Fe}_{0.25}\text{Co}_{0.25}\text{Ni}_{0.25}\text{Cu}_{0.25}$	screw	0.07 ± 0.01
	edge	0.18 ± 0.01
$\text{Fe}_{0.2}\text{Co}_{0.2}\text{Ni}_{0.2}\text{Cu}_{0.2}\text{Cr}_{0.2}$	screw	0.08 ± 0.01
	edge	0.19 ± 0.03

acoustic distortions. This explains why the composition dependence of B' can be stronger, and statistically noisier, than the composition dependence of B_0 even within a fixed lattice and slip family.

The consistently larger scatter of B' for the screw character in Table III follows from the same weighting logic. Screw motion couples predominantly through shear and therefore projects more strongly onto low-frequency transverse response, so configuration-to-configuration changes in the near-core force constant landscape translate into larger fractional changes in the infrared coupling amplitude. The ω^{-2} kernel then amplifies these changes into an enhanced variance of the thermal slope. Edge character couples more broadly in frequency because of its dilatational component, so the same chemical fluctuations are less strongly amplified in B' even when they substantially affect B_0 .

Figure 5 illustrates these general points for equiatomic AlWMo. The observed near linearity over a broad interval is consistent with the regime in which the thermally populated band satisfies $n_B(\omega) \simeq k_B T / (\hbar\omega)$ on the dominant support of the integral, while the low-temperature curvature is the controlled quantum crossover obtained by retaining the full $\coth(\beta\hbar\omega/2)$ factor rather than introducing any additional temperature-dependent parameters. The practical consequence is that once $\rho_0(\omega)$ has been computed, the entire function $B(T)$ follows analytically for all temperatures by Bose reweighting, so that thermal trends are obtained without additional dynamical simulations and with an explicit link to the infrared spectral weight that controls dissipation.

5. Memory kernel structure and mobility laws

The ensemble-averaged mobility kernel $\bar{\Gamma}(i\xi)$ is smooth, positive, and monotonically decreasing in ξ , with a finite static limit $B = \bar{\Gamma}(0)$. In all systems studied, $\bar{\Gamma}(i\xi)$ remains close to B over a low-frequency interval and then crosses over into a gradual decay across the vibrational bandwidth. This behavior implies a clean operational separation between a long-time regime in which a purely viscous mobility is accurate and a short-time regime in which history dependence matters. Rather than attributing microscopic meaning to a single crossover point, we quantify the onset of non-Markovian corrections by defining ξ_ε through $|\bar{\Gamma}(i\xi_\varepsilon) - B|/B = \varepsilon$ and the associated timescale $\tau_\varepsilon = \xi_\varepsilon^{-1}$. If the spectral content of $\dot{X}(t)$ is concentrated at $\xi \ll \xi_\varepsilon$, replacing the full kernel by its static limit introduces a relative error of order ε in the friction law.

For reduced-order modeling and stable time integration, we approximate $\bar{\Gamma}(i\xi)$ by a rational Stieltjes surrogate with positive residues,

$$\bar{\Gamma}(i\xi) \approx \sum_{m=1}^M \frac{w_m \Omega_m^2}{\xi^2 + \Omega_m^2}, \quad w_m > 0, \quad \sum_{m=1}^M w_m = B. \quad (109)$$

This form is dictated by structure rather than convenience. For a harmonic bath, the retarded friction kernel is a Stieltjes function of s^2 , so any surrogate used in time domain propagation should preserve causality and passivity; Eq. (109) enforces non-negative dissipation for arbitrary driving histories by construction. It also preserves the static moment exactly, so the long-time viscous limit is recovered without further tuning. In practice, for $M = 2$ the surrogate captures the observed curvature of $\bar{\Gamma}(i\xi)$ over the fitted window in all systems considered; increasing M typically yields near-degenerate nodes once positivity and the moment constraint are enforced. The fitted pairs (w_m, Ω_m) should therefore be read primarily as quadrature parameters defining a passive reduced order realization of the kernel over the resolved band, rather than as a spectroscopic decomposition into distinct microscopic relaxation channels.

In steady glide, the memory structure does not enter explicitly. In the linear regime, the retarded friction force per unit length is $f(t) = \int_0^\infty \Gamma(\theta) \dot{X}(t - \theta) d\theta$, so for uniform motion $\dot{X}(t) = v$ one has $f = v \int_0^\infty \Gamma(\theta) d\theta = v\hat{\Gamma}(0) = vB$. The steady-state mobility law is therefore the familiar viscous relation

$$v = \frac{b \tau_{\text{RSS}}}{B}, \quad (110)$$

with $B = \bar{\Gamma}(0)$ as tabulated. This is the expression employed in, e.g., dislocation dynamics simulations to confer a timescale to the evolution of the dislocation microstructure (see, e.g., Refs. [115,116]). We note, however, that within the present framework, this mobility law is exact, rather than phenomenological: the full frequency dependence of the kernel controls transient response but drops out of sustained uniform glide.

The regime in which Eq. (110) becomes inadequate is therefore not a large constant velocity but rapidly varying velocity, such as acceleration from rest, deceleration at obstacles, oscillatory loading, or any situation in which $\dot{X}(t)$ carries appreciable weight at frequencies $\xi \gtrsim \xi_\varepsilon$. In such a regime, the full memory kernel computed from first principles via

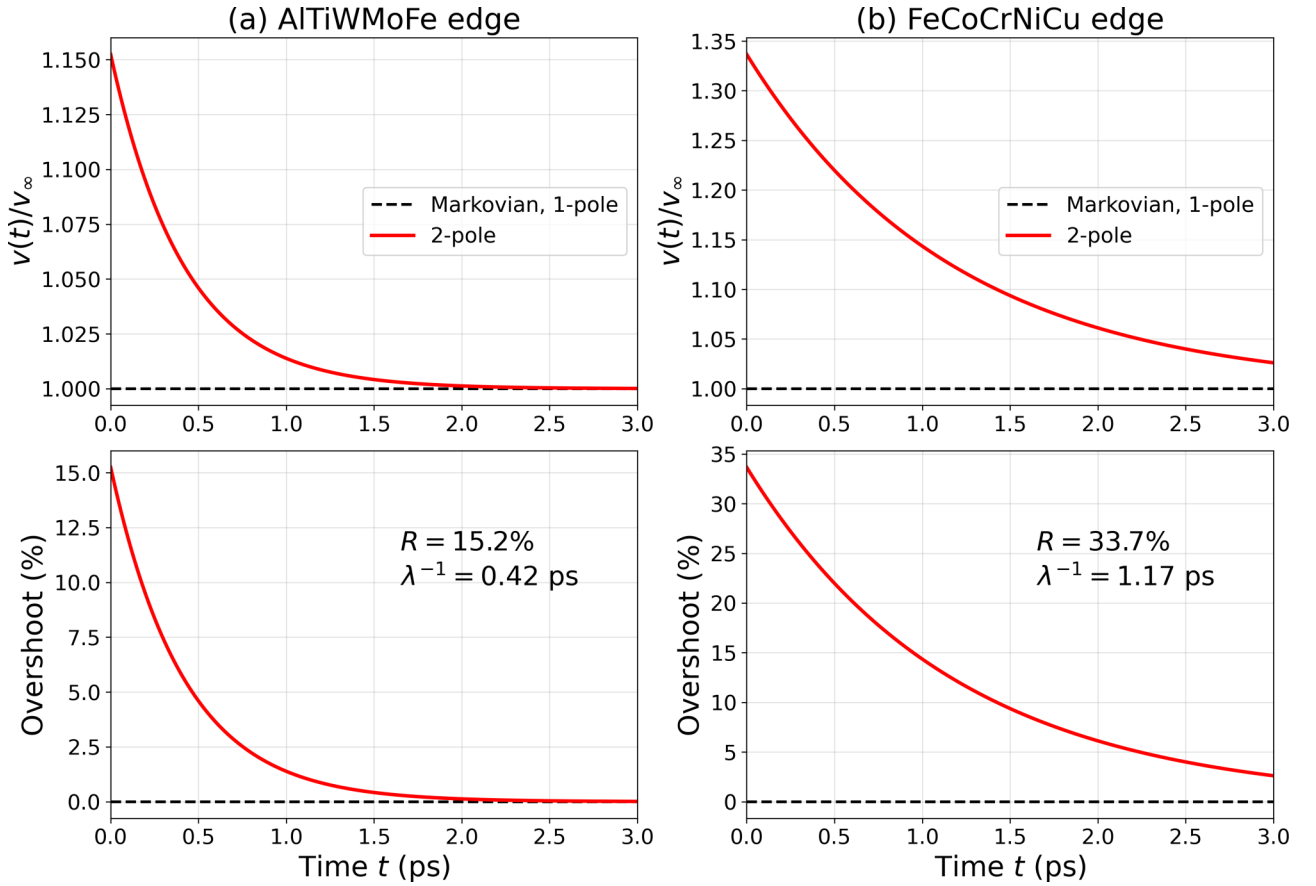


FIG. 6. Transient velocity response of edge dislocations under step-stress loading in the bcc AlTiWMoFe and fcc FeCoCrNiCu quinary systems, comparing the Markovian ($v = v_\infty$ instantaneously), one-pole ($M = 1$, degenerate with Markovian for this normalized step response), and two-pole ($M = 2$) Stieltjes mobility laws. Upper panels show $v(t)/v_\infty$; lower panels show the velocity overshoot as a percentage of v_∞ . The two-pole model predicts an initial overshoot of about 15% (bcc) and about 34% (fcc) that relaxes on a timescale $\lambda^{-1} \approx 0.4\text{--}1.2$ ps set by the bath pole structure, where $v_\infty = (b/B)\tau$, with B the per-unit line drag coefficient reported in Table I.

Eq. (110) the Stieltjes surrogate (or, indeed, the full provides a compact and structure-preserving time domain mobility law through a Markovian embedding). Introducing auxiliary friction variables $z_m(t)$, the retarded equation of motion may be written as

$$b \tau_{\text{RSS}}(t) = \sum_{m=1}^M z_m(t), \quad (111)$$

$$\dot{z}_m(t) + \Omega_m z_m(t) = w_m \Omega_m \dot{X}(t), \quad m = 1, \dots, M. \quad (112)$$

Eliminating z_m recovers the convolution with $\Gamma(t)$ corresponding to Eq. (109). In the steady state $z_m \rightarrow w_m \dot{X}$ and Eq. (110) follows immediately since $\sum_m w_m = B$. Under transient loading the z_m lag behind $\dot{X}$ and generate history dependent corrections whose accuracy is controlled by the fit error of $\bar{\Gamma}(i\xi)$ on the imaginary axis grid. The parameters (w_m, Ω_m) reported in Table I therefore constitute a complete input set for non-Markovian discrete dislocation dynamics within the linear response regime resolved by the present calculation.

To illustrate the practical consequences of the pole structure, we solve Eqs. (111)–(112) analytically for step stress loading from rest, $\tau_{\text{RSS}}(t) = \tau_0 \Theta(t)$, with $z_m(0) = 0$. This is an approximation; in practice, most loading is ramped up rather than sudden, and in most MD simulations it is noisy

and nonmonotonic. For $M = 1$ the system is algebraically degenerate: the single auxiliary variable tracks the velocity without lag, giving $v(t) = v_\infty \equiv b\tau_0/B$ for all $t > 0$, identically to the Markovian law. A single exponential kernel, while non-Markovian in form, has only one relaxation channel and therefore cannot sustain a transient under constant forcing. For $M = 2$ the Laplace inversion yields a genuine overshoot,

$$\frac{v(t)}{v_\infty} = 1 + R e^{-\lambda t}, \quad (113)$$

with

$$\lambda = \frac{\Omega_1 \Omega_2 B}{w_1 \Omega_1 + w_2 \Omega_2}, \quad R = -\frac{(\lambda - \Omega_1)(\lambda - \Omega_2)}{\Omega_1 \Omega_2},$$

and $R > 0$ since $\Omega_1 < \lambda < \Omega_2$. At $t = 0^+$ neither auxiliary variable has built up its equilibrium value, so the effective friction is less than B and the dislocation initially travels faster than its steady-state velocity; as the slow channel equilibrates the full drag is restored and $v \rightarrow v_\infty$ from above.

Figures 6 and 7 display this transient for edge and screw dislocations, respectively, in the two quinary systems. For edges, the two-pole overshoot at $t = 0^+$ is approximately 15% in bcc AlTiWMoFe and 13% in fcc FeCoCrNiCu, relaxing with time constants $\lambda^{-1} \approx 0.52$ and 0.55 ps. For screws, the effect is markedly larger: about 22% (bcc) and about 19%

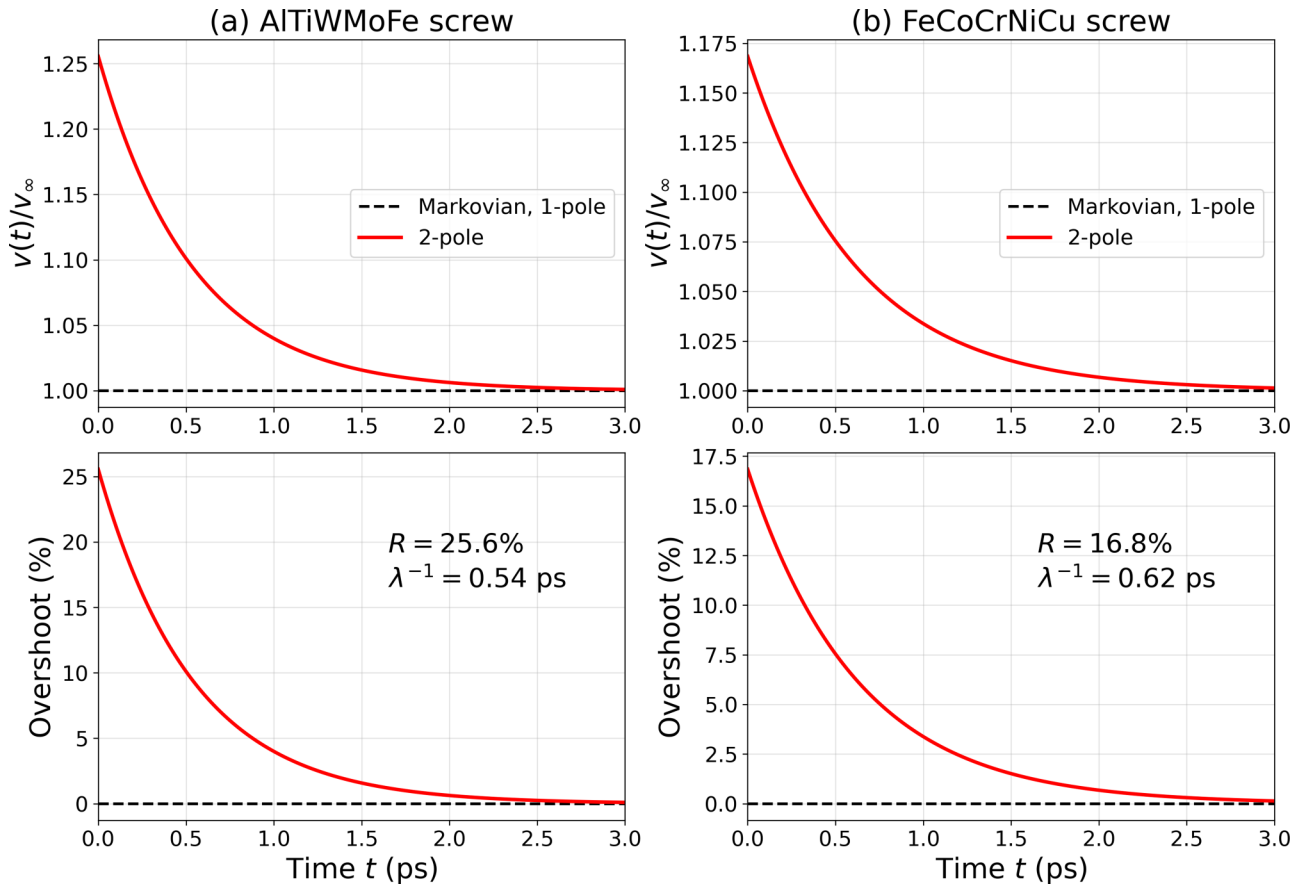


FIG. 7. As Fig. 6, but for screw dislocations. The two-pole overshoot is larger than for edges: about 26% (bcc) and about 17% (fcc), with a longer relaxation time $\lambda^{-1} \approx 0.62$ ps, reflecting the more strongly skewed weight partition toward the slow pole in screw kernels. Here $v_\infty = (b/B)\tau$, with B the per-unit line drag coefficient reported in Table I.

(fcc), with $\lambda^{-1} \approx 0.74$ ps. The enhanced screw overshoot reflects a more strongly skewed weight partition toward the slow pole ($w_1/B \approx 0.35$ for screws versus about 0.28 for edges), so that a larger fraction of the total drag is carried by the channel that is slowest to equilibrate. In both cases, the Markovian and one-pole models predict instantaneous attainment of the steady state, confirming that at least two poles are required for the Stieltjes surrogate to produce nontrivial transient dynamics under step loading.

Figure 8 extends this comparison across the ternary, quaternary, and quinary compositions within each lattice family. The relaxation time λ^{-1} is remarkably stable across compositions, varying only between 0.48 and 0.84 ps, because it is controlled by the ratio of pole frequencies to their weight partition rather than by B alone. The overshoot amplitude R , by contrast, shows clear material dependence. Within the bcc edge family R ranges from 0.10 to 0.18, while bcc screws span 0.20–0.22, with AlTiWMoFe exhibiting the largest screw overshoot despite not having the largest static drag. In the fcc edge family, adding Cr to form FeCoCrNiCu suppresses R from about 0.17 (FeCoNi, FeCoNiCu) to 0.18, reflecting a redistribution of spectral weight from the slow to the fast pole; the same composition change has almost no effect on the screw overshoot, where all three alloys cluster near $R \approx 0.19$. This character-dependent sensitivity to composition underscores that the pole structure en-

codes genuinely distinct information from the static drag B .

The subpicosecond relaxation times mean that for any discrete dislocation dynamics time step coarser than about 1 ps, the Markovian law $v = b\tau/B$ is an excellent approximation. The auxiliary variable formulation becomes important only when the dynamics resolves subpicosecond transients, as occurs in shock loading, high-frequency oscillatory driving, or the initial acceleration phase following obstacle release. In those regimes, the velocity overshoot predicted by the two-pole model is not a small correction: a 10%–22% excess velocity, sustained over a fraction of a picosecond, can influence the probability of barrier crossing and the effective mobility at short timescales.

Finally, it is important to distinguish bath memory from genuinely velocity-dependent drag. The strong increase of drag observed in driven molecular dynamics as the dislocation speed approaches the transverse sound speed arises either from resonances driven by the fixed boundaries of the MD simulation cell [117], or else from the velocity dependence that the Doppler vertex induces Kanzaki coupling itself [71]. This effect is distinct from the frequency dependence of $\bar{\Gamma}(\omega)$ at fixed coupling. Capturing it requires extending the formalism so that the coupling depends on the instantaneous velocity, while retaining the passive Stieltjes structure for the bath; this has already been done for ordered systems in

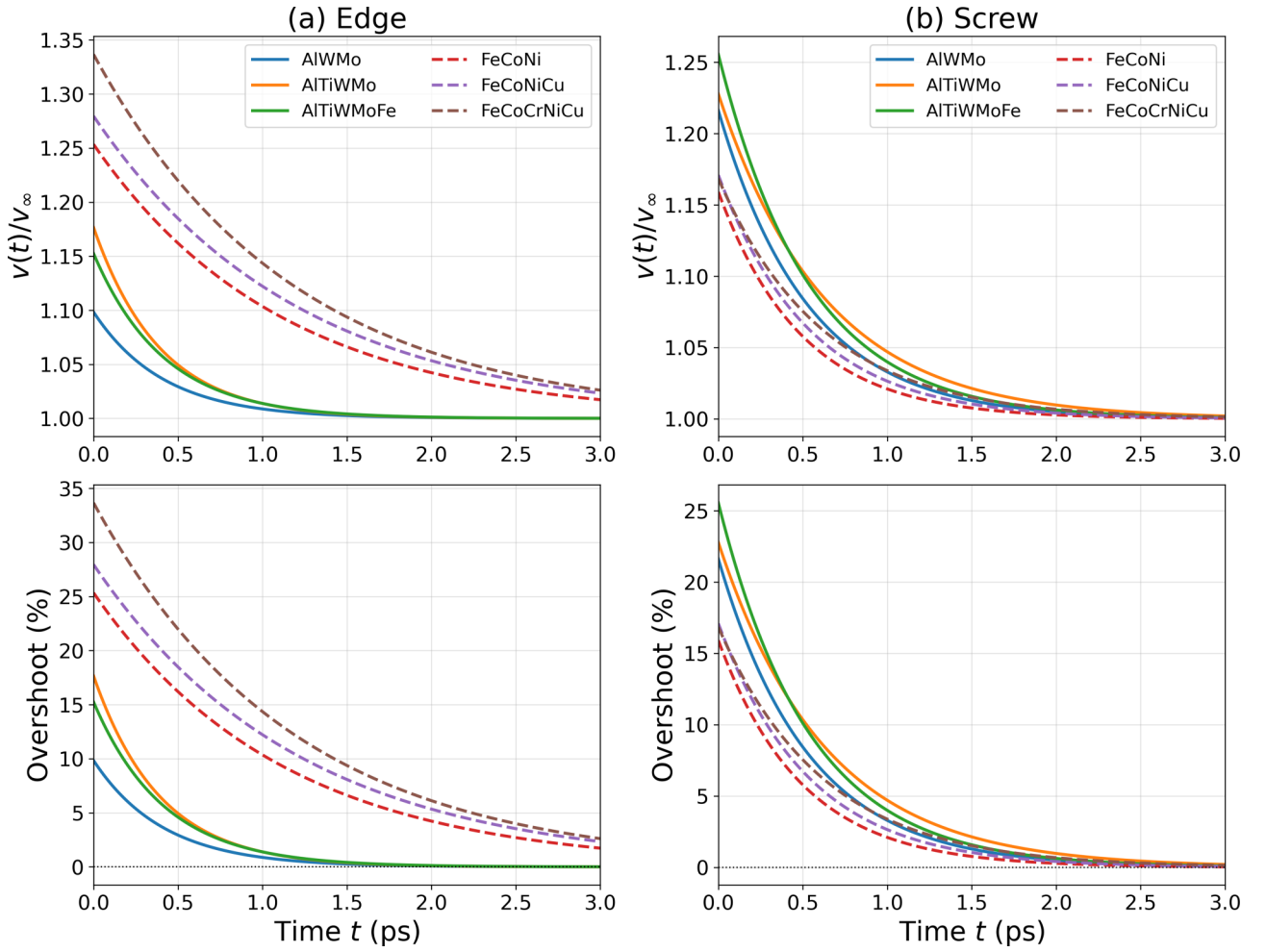


FIG. 8. Composition and character dependence of the two-pole transient velocity overshoot for edge and screw dislocations in three equimolar bcc and fcc disordered alloys under step-stress loading. All curves show $v(t)/v_\infty = 1 + \text{Re}^{-\lambda t}$ from Eq. (113). Here $v_\infty = (b/B)\tau$, with B the per-unit line drag coefficient reported in Table I.

Ref. [71] and will be the subject of future work for HEAs. The embedding in Eqs. (111) and (112) is a natural starting point for such an extension because it separates the bath dynamics, encoded by (w_m, Ω_m) , from the driving term proportional to $\dot{X}(t)$, which is precisely where a velocity-dependent coupling would enter.

6. Transferability across interatomic models and MLIP-based calculations

A central structural feature of the present formulation is that it requires only the harmonic force constant matrix and the Kanzaki driving field evaluated about a relaxed configuration. The mobility kernel is then obtained from the embedded lattice Green's function and the associated projected spectral measure. No driven atomistic dynamics enters at any stage. The framework therefore applies without modification to force constants obtained from classical EAM potentials, from MLIPs, or from conformal field theory (CFT), provided that the force constants are computed consistently with the relaxed atomic state on which the Kanzaki field is defined.

This separation between lattice dynamics and defect motion is especially valuable in chemically complex alloys. In

high-entropy systems, direct molecular dynamics sampling of dislocation glide with accurate interaction models is computationally prohibitive, particularly if one seeks statistically meaningful averages over chemical realizations. A conventional extraction of drag coefficients would require repeated nonequilibrium simulations across many chemically distinct supercells, typically at strain rates far above experimental conditions. Here, that procedure is replaced by a single equilibrium force constant calculation per configuration, after which the entire frequency-dependent mobility kernel, together with its static drag and thermal slope, follows analytically from the projected spectral measure.

We illustrate this transferability by repeating the embedding calculation for equiatomic bcc $\text{Al}_{0.33}\text{W}_{0.33}\text{Mo}_{0.33}$ using a Multilayer Atomic Cluster Expansion (MACE) MLIP [72] and by applying the same workflow to the quinary $\text{Al}_{0.2}\text{W}_{0.2}\text{Mo}_{0.2}\text{Ti}_{0.2}\text{Cr}_{0.2}\text{Cr}_{0.2}$ alloy for which no reliable EAM description is available. For $\text{Al}_{0.33}\text{W}_{0.33}\text{Mo}_{0.33}$ the MLIP-based drags are systematically larger than those obtained from an EAM description (e.g., ≈ 110 vs $\approx 328 \mu\text{Pa s}$ for edges), while the screw-edge hierarchy, the coherence ratios, and the pole structure of the kernel are otherwise pre-

served (see Table I). This indicates that the interatomic model primarily modulates the magnitude of dissipation, without substantially altering the structural form of the mobility law.

The origin of this increase is found in our expression for the drag kernel [Eq. (21)], which is a functional of the projected spectral density induced by the Kanzaki vertex. At low temperature, it weights that measure by $\rho(\omega)/\omega$, with the thermal slope introducing an even stronger $\rho(\omega)/\omega^2$ weighting. It is therefore natural to interpret interatomic model dependence through a decomposition of the harmonic operator into a mean medium plus disorder fluctuations. Writing the configuration-dependent dynamical matrix as $D = \bar{D} + \delta D$, an effective medium calculation corresponds to replacing D by $\bar{D}$ at the outset, hence retaining only the contribution controlled by the first moment of the harmonic operator. The full calculation retains, in addition, the non-negative fluctuation correction generated by δD through the projected resolvent. This variance contribution is governed by higher-order disorder statistics of the force constants as sampled by the Kanzaki field, and it is the channel through which local environment dependence and mass stiffness correlations enter the dissipation.

Since classical EAM parametrizations are commonly constrained primarily by averaged equilibrium and elastic observables [118,119], they can reproduce the mean harmonic response while providing a less faithful representation of the environment dependent force constant disorder that controls the fluctuation contribution in random alloys, where environmental disorder is intrinsic to the force constant sum-rule structure [88]; this limitation is consistent with the broader observation that empirical potentials frequently require dedicated phonon-oriented optimization to reproduce interatomic force constant information relevant to vibrational properties [119]. In turn, MLIPs trained to first principles data capture a richer configuration sensitivity of the harmonic couplings, which increases the fluctuation content of δD and thereby enhances the variance contribution, while leaving the effective medium part comparatively unchanged when the mean stiffness landscape is similar. This separation is further emphasized by noting that the effective medium drag coefficient obtained from the EAM and MLIP force constants are close (i.e., ≈ 50 vs $69 \mu\text{Pa s}$ for screw dislocations in AlWMo) despite the actual drag being much larger in the latter: once disorder fluctuations are suppressed by the replacement $D \mapsto \bar{D}$, both descriptions reduce to essentially the same mean harmonic medium, consistent with comparable long-wavelength elastic response and similar locations of the dominant poles of the embedded Green's function. The substantial difference in the full drags is therefore attributable to the fluctuation correction carried by δD , rather than to a change in the underlying effective elastic background.

Methodologically, the embedding and spectral framework provides a route to dislocation mobility parameters with near first principles fidelity at a cost far below that of direct nonequilibrium molecular dynamics performed with the same interaction model. Once the force constants and Kanzaki field are available, the drag, its thermal slope, and a structure-preserving reduced-order memory kernel follow without further dynamical sampling. This makes it practical to

deploy MLIP, and in favorable cases DFT, force constants for chemically complex alloys where direct dynamical averaging would be infeasible.

7. Implications for the mechanical response of HEAs at high strain rates

A persistent heuristic in the high-strain-rate literature on single-phase HEAs is that increasing chemical complexity should raise the drag-controlled resistance to motion and thereby promote dynamic strengthening. In the present formulation, there is no basis for such monotonicity. The static coefficient B and the thermal slope B' are spectral moments of the line-projected measure $\rho_0(\omega)$ filtered by the Kanzaki vertex. Composition enters only through how local chemistry reshapes this projected spectral weight. Since dissipation depends on the configurational average of squared couplings, the drag is controlled by the infrared-weighted statistics of the local core environment rather than by bulk elastic descriptors. Adding species may increase or decrease the relevant projected weight, depending on how mass and stiffness fluctuations redistribute low-frequency coupling near the core. The nonmonotone trends reported in Tables I and III are therefore the generic outcome of a local spectral mechanism, not anomalies relative to a host-based scaling.

The importance of this point becomes clear once one recalls the well-established rate hierarchy of crystal plasticity. A substantial experimental literature shows that, above strain rates of order 10^3 – 10^4 s^{-1} , the rate-limiting mechanism in many metals crosses over from thermally activated barrier crossing to phonon drag-controlled glide [120–124]. In this regime, the Peierls barrier is effectively surmounted on the timescale of loading, and the flow stress acquires a viscous contribution proportional to the drag coefficient through the mobility law

$$v = \frac{b \tau_{\text{RSS}}}{B(T)}, \quad \dot{\gamma} = \rho_m b v.$$

Plastic resistance then scales directly with $B(T)$ at a fixed mobile dislocation density [125]. A characteristic signature of this regime is the observed softening with increasing temperature under dynamic loading [121]: as the temperature rises, the drag increases approximately linearly, $B(T) \simeq B_0 + B'T$, so that at fixed imposed strain rate the required stress adjusts through the viscous relation rather than through increased work hardening. The high rate plastic response is therefore controlled by the same spectral object that determines B and B' in the present theory.

It follows immediately that if alloying does not guarantee an increase of B , then increasing chemical complexity does not guarantee enhanced dynamic strengthening once drag-dominated flow sets in. Compositions that reduce the infrared projected weight will exhibit lower viscous resistance at a given strain rate, enabling faster slip and enhancing the competition between plastic dissipation and adiabatic heating. In contrast, compositions that enhance the projected spectral weight increase viscous resistance and may delay localization. The decisive quantity is therefore not the number of principal elements but how their local chemical statistics modify the dislocation-phonon coupling in the infrared.

This perspective helps rationalize the diversity of experimental trends reported under extreme loading. Instances in which dynamic response is weaker than expected, whether through muted strain rate sensitivity, negative rate sensitivity in specific temperature windows, or early adiabatic shear localization, are consistent with the absence of a monotone drag enhancement with disorder. Conversely, alloys that retain strong resistance to shear banding at high rate can be interpreted as compositions in which the projected infrared weight remains large. The framework developed here makes these distinctions quantitative by computing $B(T)$ and B' directly from the disorder-averaged spectral density, thereby linking high-rate mechanical response to a well-defined microscopic object rather than to heuristic measures of lattice distortion or chemical complexity.

A growing body of high-rate data is at least consistent with the need for such nonmonotone microscopic trends. For instance, the quinary CrMnFeCoNi Cantor alloy has been found to be less ballistic resistant than the four-component CrFeCoNi subsystem [126], a result that already contradicts any monotone “more elements, better dynamic performance” narrative. From the present perspective, this is unsurprising, because adding a species modifies the configuration dependent spectral density and coupling statistics in a way that need not increase the infrared weight controlling B and B' . Split Hopkinson pressure bar measurements on fcc HEAs frequently report small strain rate sensitivity exponents $m \lesssim 0.01$ [127], values that are negligible by the standards of concentrated solid solutions and sit below what a naive lattice distortion argument might suggest. Negative strain rate sensitivity has also been reported in $\text{Al}_{0.1}\text{CoCrFeNi}$ at intermediate temperatures [128] and in nanocrystalline CoCrFeMnNi [129], indicating regimes in which the dynamic response can invert once other rate-controlling channels become active. High rate compression of $\text{Al}_{0.3}\text{CoCrFeNi}$ has been analyzed within a Johnson–Cook form in which an explicit thermal softening term is required to capture the high-velocity response, demonstrating that adiabatic heating can enter as a leading term even in alloys often advertised as shear-localization resistant [130].

The picture extends beyond fcc systems. In bcc refractory HEAs, spall strengths are often reported as lower than those of fcc counterparts, and in TiZrNbV fine-grained material can perform worse than coarse-grained under plate impact, with adiabatic shear bands implicated in brittle dynamic failure at 10^3 – 10^4 s^{-1} [131]. Precipitation-strengthened fcc HEAs can also become susceptible to adiabatic shear through dissolution of coherent L_{12} nanoprecipitates under dynamic loading [132], a mechanism that undermines precisely the microstructural strategy used to compensate for the low intrinsic yield strength of single-phase fcc HEAs. Yet single-phase fcc HEAs themselves can be strongly resistant, for example, the Cantor alloy sustains shear strains of order $\gamma \approx 7$ before adiabatic shear band formation [133]. The diversity of these outcomes is not naturally reconciled with any model in which dynamic dissipation scales monotonically with chemical complexity.

The present formulation makes the relevant competition quantitative and composition-specific. The objects we compute, $\rho_0(\omega)$, $\bar{\Gamma}(\omega)$, and their variances, are microscopic inputs

that determine whether a given composition exhibits enhanced or muted drag-controlled strengthening, and whether that strengthening can plausibly outrun adiabatic softening for a given loading history. This is difficult to extract from driven molecular dynamics in a systematic way for HEAs, because the rates required to infer B are extreme, and the need for configurational statistics multiplies the cost, while the simulation output does not in itself identify how dissipation is distributed across vibrational modes or how that spectral weight redistributes with chemistry. Here, the same equilibrium spectral calculation produces $B(T)$ and B' for each configuration, together with controlled uncertainty estimates, while isolating the local core environment as the causal source of the trend. In particular, because the dominant contribution to drag in these alloys is a variance term discarded by homogenized descriptions, there is no reason to expect a monotone correlation between bulk-averaged descriptors and dynamic response.

The present theory is harmonic in the lattice degrees of freedom. The retarded Green’s function entering the kernel is constructed from force constants evaluated about a mechanically relaxed configuration, so temperature enters through the phonon occupation factors, while thermal expansion, phonon-phonon scattering, anharmonic frequency shifts, and nonlinear core fluctuations are not included explicitly. In an anharmonic extension, the harmonic spectral measure would be replaced by a temperature-dependent interacting spectral function, with finite linewidths and shifted spectral weight, as proposed for the ordered crystal case by Gurrutxaga-Lerma [71]. These effects would recalibrate the inverse moments that determine the drag and its thermal slope, particularly at high temperature or near mechanical instabilities. If anharmonicity is incorporated through an effective surrounding bath, the natural choice would be a cluster extension of the phonon effective medium, including dynamical cluster or typical medium formulations, since these retain nonlocal disorder correlations and can capture disorder-induced phonon localization through typical rather than only arithmetic spectral functions [55,56,58]. Such a cluster medium could improve the far-field bath in the present embedding construction, but it would not remove the need to retain the near-core Kanzaki source and inner Green’s function configuration by configuration before averaging. The central conclusions, however, do not rely on harmonicity itself: the noncommutativity between configurational averaging and homogeneous effective medium construction follows from the quadratic dependence of the dissipation kernel on the configuration-dependent source and retarded response, and would persist for any causal, passive lattice spectral function.

VIII. CONCLUSIONS

This work gives a first-principles answer to what phonon drag is in a chemically disordered crystal. Phonon drag is the retarded backaction of the lattice on a moving dislocation, and its fundamental descriptor is a causal memory kernel rather than a scalar viscosity. The drag coefficient B used in continuum mobility laws is the zero-frequency limit of this kernel, not an empirical input. Within the harmonic approximation, the kernel and its associated spectral density are equilibrium objects, so steady glide, transient response, and the full

temperature dependence follow from the same calculation rather than from protocol-dependent driven simulations. The central outcome is therefore both conceptual and practical: dislocation drag in a chemically complex alloy can be formulated as a projected spectral property of the lattice, computed at equilibrium, and then passed directly to mesoscale mobility laws.

Methodologically, we have constructed a configuration-resolved influence functional for dislocation glide in a disordered alloy. For each chemical realization $\mathcal{C}$, the Keldysh–Kanzaki construction integrates out the harmonic lattice exactly and produces an effective action whose content is exhausted by a retarded kernel and its Keldysh partner fixed by fluctuation dissipation. The lattice dynamics and the Kanzaki source are temperature independent within this approximation, so finite temperature enters only through Bose occupation factors in the symmetrized correlator. In practical terms, one equilibrium phonon computation yields the spectral density $\rho_{\mathcal{C}}(\Omega)$ and therefore the entire mobility kernel, while quenched averaging can be performed directly at the level of kernels or spectral measures in a manner consistent with linearity of the influence functional. This is the step that makes the framework suitable for high-entropy alloys: the calculation retains configuration-by-configuration fluctuations before averaging, rather than replacing the alloy by a homogeneous medium at the outset.

The physical picture that follows is that alloying changes drag primarily by reshaping and randomizing the dislocation phonon coupling near the core, not by a small perturbation of a host-based descriptor. In an ordered crystal, the coupling is translationally coherent and radiated phonons retain phase coherence into the far field, so dissipation is delocalized. In a concentrated alloy, the same phonons experience strong scattering from mass and force constant disorder on near-atomic length scales, concentrating energy transfer to the vicinity of the core where Kanzaki fields and strain gradients are largest. In this setting, the disorder average that enters drag is inherently quadratic in the configuration dependent coupling, and this is precisely where homogenized descriptions fail. The calculations show that this is not a minor correction: in the fcc and bcc alloys studied here, the variance of the local coupling is the dominant contribution to the drag enhancement relative to homogeneous effective media.

We have shown through a mathematical theorem that failure is structural, not a matter of fit quality. Drag, as a positive quadratic functional of the Kanzaki couplings, depends on $\langle |g_{\nu\mathcal{C}}|^2 \rangle_{\mathcal{C}}$, whereas any effective medium that replaces the alloy by an averaged crystal computes $|\langle g_{\nu\mathcal{C}} \rangle_{\mathcal{C}}|^2$. The gap between these objects is the variance contribution $\langle |g|^2 \rangle_{\mathcal{C}} - |\langle g \rangle_{\mathcal{C}}|^2 \geq 0$, which cannot be recovered by refining the effective medium because it is absent by construction. In the systems studied here, virtual crystal style approaches systematically underestimate B , collapse the screw to edge contrast, and suppress composition-dependent contributions to drag. Thus, the relevant distinction is not between a poor and a good average crystal, but between averaging the mobility kernel itself and constructing a mobility kernel only after the chemical fluctuations have already been removed.

The same viewpoint clarifies what becomes of classical expectations, such as Leibfried-type scaling of the disloca-

tion drag. The host-based result where the dominant thermal contribution is linear in T is recovered naturally as the high-temperature asymptotics of Bose reweighting, but the prefactor is not determined by a small set of bulk descriptors. It is determined by an infrared-weighted spectral moment of the disorder-averaged spectral measure filtered by the dislocation phonon vertex, hence it is sensitive to chemistry and core environment in a way that bulk sound speeds and Grüneisen parameters do not encode. Alloying, therefore, need not produce monotone trends in drag even within a fixed lattice and slip family, and changes in chemical complexity can either enhance or suppress the projected spectral weight that controls dissipation. This explains why the drag trends obtained here are chemically specific rather than simply increasing with the number of principal elements.

The comparison between interatomic descriptions reinforces this conclusion. The effective media obtained from EAM and machine-learned interatomic potentials are close when disorder fluctuations are suppressed, indicating that the mean harmonic backgrounds are similar. The full configuration-resolved drags, however, differ more substantially, because the interatomic model changes the fluctuation statistics of the force constants and their coupling to the Kanzaki source. The role of a higher fidelity interatomic model is therefore not to alter the formal mobility law, but to provide a more faithful projected spectral measure for the chemically fluctuating lattice sampled by the dislocation core.

For modeling practice, the output of the theory is immediately usable. In steady glide, the mobility reduces exactly to the viscous law $v = b \tau_{\text{RSS}}/B(T)$, with $B(T)$ obtained for all temperatures by Bose reweighting of the same spectral density. When the dislocation velocity varies rapidly, the full kernel provides a controlled non-Markovian mobility law. A positive rational Stieltjes surrogate fitted to $\bar{\Gamma}(i\xi)$ preserves causality and passivity and can be implemented as a small set of auxiliary ordinary differential equations driven by the glide velocity, eliminating the need to store velocity history. No calibration to driven dynamics is required once the spectral density has been computed, and the tabulated pole parameters therefore constitute an input set for discrete dislocation dynamics that goes beyond a single drag constant while remaining computationally negligible at the mesoscale.

The broader implication is that disorder-controlled mobility can now be treated as a local, spectral, and statistically well-defined materials property. The same construction applies without modification to random alloys, SQS cells, short-range-ordered ensembles, cluster expansion samples, and experimentally constrained chemical configurations, because these choices change only the probability measure over realizations. The framework also provides a natural route to mobility databases based on DFT or machine-learned force constants, at a cost far below that of repeated nonequilibrium simulations over large chemical ensembles. In this sense the present work replaces phenomenological drag coefficients by a microscopically defined projected spectral measure, identifies fluctuations of the dislocation phonon coupling as the dominant control parameter in concentrated alloys, and provides a structure-preserving bridge from atomistic lattice dynamics to mesoscale plasticity in chemically complex materials.

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Views and opinions expressed are, however, those of the author(s) only and do not necessarily reflect those of the European Union or HADEA. Neither the European Union nor HADEA can be held responsible for them.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: DETAILS OF SEC. II CONSTRUCTION

This appendix collects the algebraic and constructional details underlying the compact formulation used in Sec. II. The main text keeps the configuration-resolved Hamiltonian, the Kanzaki interaction, the diagonal phonon Hamiltonian, and the influence action, while the derivations below make explicit how these objects are obtained.

1. Discrete Volterra construction and Kanzaki reduction

On the discrete lattice, the defect is represented by a Volterra slip configuration X and the associated displacement discontinuity across a slip surface S . Let δ_α label the nearest-neighbor bond vectors and let $(x_{\mathbf{R}}, y_{\mathbf{R}}, z_{\mathbf{R}})$ denote the Cartesian coordinates of site $\mathbf{R}$. We take the slip plane to be $y = 0$ and the slip front to lie at $x = X$. Bonds whose midpoints lie behind the front and cross the slip plane are selected by the bond-crossing indicator

$$c_\alpha(\mathbf{R}; X) = \frac{1}{2} \left[\text{sgn} \left(y_{\mathbf{R}} + \frac{\delta_{\alpha,y}}{2} \right) - \text{sgn} \left(y_{\mathbf{R}} - \frac{\delta_{\alpha,y}}{2} \right) \right] \Theta(X - x_{\mathbf{R}}), \quad (\text{A1})$$

which is nonzero only for bonds that cross the slip plane at $y = 0$ and lie in the wake $x_{\mathbf{R}} < X$ of the front. For bonds whose midpoint lies exactly on the slip plane we take $\text{sgn}(0) = 0$, so that such measure zero cases are assigned to neither half-space; this convention has no effect on the long-wavelength limit.

The discrete Volterra displacement $u_i^V(\mathbf{R}; X; C)$ is defined by the bond jump condition

$$u_i^V(\mathbf{R} + \delta_\alpha; X; C) - u_i^V(\mathbf{R}; X; C) = B_i c_\alpha(\mathbf{R}; X), \quad (\text{A2})$$

which implements a slip of magnitude B_i across the bonds cut by the Volterra construction and leaves all other bonds continuous. In a coarse-grained notation, one can write the jump across the slip surface S as

$$[u_i^V(\mathbf{R}; X; C)]_S = B_i \Psi(\mathbf{R}; X), \quad (\text{A3})$$

with

$$\Psi(\mathbf{R}; X) \equiv \sum_\alpha c_\alpha(\mathbf{R}; X), \quad (\text{A4})$$

so that Ψ is the site resolved slip indicator induced by the bond-crossing pattern. In the long-wavelength limit, u^V converges to the Volterra displacement of continuum elasticity for a straight dislocation with Burgers vector $\mathbf{B}$.

Fourier transforming the bond indicator gives the bond-resolved slip form factor

$$\Psi_\alpha(\mathbf{q}; X) = e^{-iq_x X} S_\alpha(\mathbf{q}_\parallel) \frac{2i \sin\left(\frac{q_y \delta_{\alpha,y}}{2}\right)}{q_x + i0^+}, \quad (\text{A5})$$

where $\mathbf{q}_\parallel = (q_x, 0, q_z)$ and $S_\alpha(\mathbf{q}_\parallel)$ is an in-plane structure factor encoding the core regularization. For the formal developments in the main text it is sufficient that $S_\alpha(\mathbf{q}_\parallel)$ is smooth, respects the point group of the slip plane, and satisfies $S_\alpha(\mathbf{0}) = 1$.

The relaxed slip displacement satisfies

$$\sum_{\mathbf{R}'} \Phi_{ij}^{(C)}(\mathbf{R}, \mathbf{R}') u_j^{\text{slip}}(\mathbf{R}'; X; C) = f_i^K(\mathbf{R}; X; C), \quad (\text{A6})$$

which reduces to Eq. (3) when $u^{\text{slip}} = u^V$. The fluctuation field in Eq. (4) contains thermal and quantum fluctuations around the static slip field and satisfies

$$\langle u_i^{\text{ph}}(\mathbf{R}, t; C) \rangle = 0. \quad (\text{A7})$$

Inserting the displacement split in Eq. (4) into Eq. (1) gives

$$H_{\text{ph}}^{(C)}[u] = H_{\text{ph}}^{(C)}[u^{\text{ph}}] + H_{\text{stat}}^{(C)}[X] + H_{\text{mix}}^{(C)}[X, u^{\text{ph}}], \quad (\text{A8})$$

where $H_{\text{ph}}^{(C)}[u^{\text{ph}}]$ has the same quadratic form as Eq. (1) with u replaced by u^{ph} , $H_{\text{stat}}^{(C)}[X]$ is a static elastic energy, and

$$H_{\text{mix}}^{(C)}[X, u^{\text{ph}}] = \sum_{\mathbf{R}, \mathbf{R}'} u_i^{\text{slip}}(\mathbf{R}; X; C) \Phi_{ij}^{(C)}(\mathbf{R}, \mathbf{R}') u_j^{\text{ph}}(\mathbf{R}'; C). \quad (\text{A9})$$

Using Eq. (A6), the mixed term reduces to

$$H_{\text{mix}}^{(C)}[X, u^{\text{ph}}] = \sum_{\mathbf{R}, i} f_i^K(\mathbf{R}; X; C) u_i^{\text{ph}}(\mathbf{R}; C). \quad (\text{A10})$$

This is the source coupling quoted in Eq. (5).

2. Normal-mode conventions

For each configuration C , the mass-weighted eigenvectors $\tilde{e}_i^{(vC)}(\mathbf{R})$ satisfy [135, 136]

$$\sum_{\mathbf{R}', j} \frac{\Phi_{ij}^{(C)}(\mathbf{R}, \mathbf{R}')}{\sqrt{M_C(\mathbf{R})M_C(\mathbf{R}')}} \tilde{e}_j^{(vC)}(\mathbf{R}') = \omega_{vC}^2 \tilde{e}_i^{(vC)}(\mathbf{R}), \quad (\text{A11})$$

with the orthonormality condition

$$\sum_{\mathbf{R},i} \tilde{e}_i^{(\nu C)}(\mathbf{R}) \tilde{e}_i^{(\mu C)}(\mathbf{R}) = \delta_{\nu\mu}. \quad (\text{A12})$$

The physical eigenvectors are

$$e_i^{(\nu C)}(\mathbf{R}) = \frac{\tilde{e}_i^{(\nu C)}(\mathbf{R})}{\sqrt{M_C(\mathbf{R})}}, \quad (\text{A13})$$

and the fluctuation field admits the mode expansion

$$u_i^{\text{ph}}(\mathbf{R}) = \sum_{\nu} \sqrt{\frac{\hbar}{2M_{\text{ref}}\omega_{\nu C}}} e_i^{(\nu C)}(\mathbf{R}) (a_{\nu C} + a_{\nu C}^{\dagger}), \quad (\text{A14})$$

where $a_{\nu C}$ and $a_{\nu C}^{\dagger}$ annihilate and create quanta of the ν th normal mode of the harmonic lattice for configuration C and obey

$$[a_{\nu C}, a_{\mu C}^{\dagger}] = \delta_{\nu\mu}, \quad [a_{\nu C}, a_{\mu C}] = [a_{\nu C}^{\dagger}, a_{\mu C}^{\dagger}] = 0.$$

The subscript C emphasizes that the mode frequencies, eigenvectors, and mode operators depend on the particular chemical realization through the masses and force constants. The choice of M_{ref} fixes only the convention in Eq. (A14); it cancels from observables.

3. Contour action and Gaussian integration

For a fixed disorder configuration C , the closed time contour generating functional is

$$\begin{aligned} \mathcal{Z}_C = & \int \mathcal{D}X_+ \mathcal{D}X_- \mathcal{D}u_+^{\text{ph}} \mathcal{D}u_-^{\text{ph}} \\ & \times \exp \left\{ \frac{i}{\hbar} (S_{\text{dis}}[X_+] - S_{\text{dis}}[X_-] + S_{\text{ph}}^{(C)}[u_+^{\text{ph}}] - S_{\text{ph}}^{(C)}[u_-^{\text{ph}}] \right. \\ & \left. + S_{\text{int}}^{(C)}[X_+, u_+^{\text{ph}}] - S_{\text{int}}^{(C)}[X_-, u_-^{\text{ph}}] \right\}, \quad (\text{A15}) \end{aligned}$$

where $S_{\text{ph}}^{(C)}[u] = \frac{1}{2} \int_C dt (\dot{u}^T M^{(C)} \dot{u} - u^T \Phi^{(C)} u)$ is the quadratic contour action corresponding to $H_{\text{ph}}^{(C)}$, and, since $H_{\text{int}}^{(C)}$ depends only on coordinates, $S_{\text{int}}^{(C)}[u, X] = - \int_C dt H_{\text{int}}^{(C)}(u(t), X(t))$.

Since $H_{\text{ph}}^{(C)}$ is quadratic and $H_{\text{int}}^{(C)}$ is linear in u^{ph} , the integrals over $u_{\pm}^{\text{ph}}$ are Gaussian and can be carried out exactly. This defines an influence action,

$$\begin{aligned} \mathcal{Z}_C = & \int \mathcal{D}X_+ \mathcal{D}X_- \\ & \times \exp \left\{ \frac{i}{\hbar} (S_{\text{dis}}[X_+] - S_{\text{dis}}[X_-] + S_{\text{infl}}^{(C)}[X_+, X_-]) \right\}, \quad (\text{A16}) \end{aligned}$$

where $S_{\text{infl}}^{(C)}$ collects the bath-induced contributions. The explicit retarded and Keldysh kernels appearing in Eq. (11) are the configuration-resolved analogs of the ordered kernels, obtained by replacing the ordered frequencies, eigenvectors, and mode couplings with $\{\omega_{\nu C}, e^{(\nu C)}, g_{\nu C}\}$.

APPENDIX B: CONFIGURATION-RESOLVED KELDYSH KERNELS FOR THE KANZAKI PHONON BATH

In this appendix we derive the configuration-resolved Keldysh kernels that enter the effective dislocation action when the dislocation couples linearly to the Kanzaki phonon bath of Sec. II A. Throughout, we work at a fixed chemical configuration C and use the mode representation introduced in Eqs. (7) and (8). The configurational average over C that defines the effective high-entropy alloy kernels is performed only at the end.

For a given C , the phonon and interaction Hamiltonians read

$$H_{\text{ph}}^{(C)} = \sum_{\nu} \hbar \omega_{\nu C} \left(a_{\nu C}^{\dagger} a_{\nu C} + \frac{1}{2} \right), \quad (\text{B1})$$

$$H_{\text{int}}^{(C)}[X] = - \sum_{\nu} g_{\nu C}(X) (a_{\nu C} + a_{\nu C}^{\dagger}), \quad (\text{B2})$$

where ν labels the normal modes of $H_{\text{ph}}^{(C)}$, with frequencies $\omega_{\nu C}$ and eigenvectors $e^{(\nu C)}$ satisfying Eq. (A11), and the Kanzaki mode couplings $g_{\nu C}(X)$ are given by Eq. (9). The dislocation coordinate $X(t)$ enters only through $g_{\nu C}(X)$; the purely dislocation part $H_{\text{dis}}[X, P_X; C]$ plays no role in the construction of the bath kernels and will be kept implicit.

1. Keldysh influence functional and force kernels

We use the real-time Keldysh functional integral with forward and backward fields $X^{\pm}(t)$ and $a_{\nu C}^{\pm}(t)$. The configuration-resolved generating functional is

$$\begin{aligned} \mathcal{Z}_C = & \int \mathcal{D}X^+ \mathcal{D}X^- \prod_{\nu} \mathcal{D}a_{\nu C}^+ \mathcal{D}a_{\nu C}^- \\ & \times \exp \left\{ \frac{i}{\hbar} (S_{\text{dis}}[X^+] - S_{\text{dis}}[X^-] + S_{\text{ph}}^{(C)}[a^+] - S_{\text{ph}}^{(C)}[a^-] \right. \\ & \left. + S_{\text{int}}^{(C)}[X^+, a^+] - S_{\text{int}}^{(C)}[X^-, a^-] \right\}, \quad (\text{B3}) \end{aligned}$$

where $S_{\text{ph}}^{(C)}$ is the quadratic action associated with Eq. (B1) and

$$S_{\text{int}}^{(C)}[X^{\pm}, a^{\pm}] = - \int dt H_{\text{int}}^{(C)}[X^{\pm}(t), a^{\pm}(t)]. \quad (\text{B4})$$

The phonon modes form a Gaussian bath, so the path integral over $a_{\nu C}^{\pm}$ can be carried out exactly, yielding an influence functional $\mathcal{F}_C[X^+, X^-]$. Introducing classical and quantum components

$$X^c(t) = \frac{X^+(t) + X^-(t)}{2}, \quad X^q(t) = X^+(t) - X^-(t), \quad (\text{B5})$$

the effective action can be written in the standard form

$$\begin{aligned} S_{\text{eff}}^{(C)}[X^c, X^q] = & S_{\text{dis}}[X^c, X^q] + \int dt X^q(t) F_{\text{det}}^{(C)}[X^c](t) \\ & - \frac{1}{2} \int dt \int dt' X^q(t) \mathcal{D}_C^R(t-t') X^c(t') \\ & - \frac{i}{2} \int dt \int dt' X^q(t) \mathcal{N}_C(t-t') X^q(t'). \quad (\text{B6}) \end{aligned}$$

Here, $F_{\text{det}}^{(C)}$ is the deterministic phonon-mediated force, while $\mathcal{D}_C^R$ and $\mathcal{N}_C$ are the retarded and noise kernels generated by the Kanzaki bath at fixed disorder configuration. They are determined by the microscopic force operator conjugate to X .

The force operator is defined as

$$F_X^{(C)}(t) = - \left. \frac{\partial H_{\text{int}}^{(C)}[X]}{\partial X} \right|_{X=X^c(t)}, \quad (\text{B7})$$

evaluated on the classical branch $X^c(t)$. The Keldysh derivation leading to Eq. (B6) is identical to that given in Sec. II, with the electronic operators replaced by the phonon operators a_{vC} and the configurational average restricted to a single realization C . The two kernels can be written directly in terms of equilibrium force correlators at fixed C :

$$\mathcal{D}_C^R(t) = \frac{i}{\hbar} \theta(t) \langle [F_X^{(C)}(t), F_X^{(C)}(0)] \rangle_C, \quad (\text{B8})$$

$$\mathcal{N}_C(t) = \frac{1}{\hbar} \langle \{F_X^{(C)}(t), F_X^{(C)}(0)\} \rangle_C / 2, \quad (\text{B9})$$

where the expectation value is taken in the thermal ensemble of $H_{\text{ph}}^{(C)}$ and $F_X^{(C)}(t)$ evolves with $H_{\text{ph}}^{(C)}$.

2. Force-based Keldysh kernels at fixed configuration

For each configuration C , the Kanzaki field $f_i^K(\mathbf{R}; X; C)$ defines a configuration-resolved force operator

$$F_X^{(C)}(t) = - \sum_{\mathbf{R}, i} [\partial_X f_i^K(\mathbf{R}; X; C)] u_i(\mathbf{R}, t; C), \quad (\text{B10})$$

with $u_i(\mathbf{R}, t; C)$ evolving under the harmonic Hamiltonian $H_{\text{ph}}^{(C)}$ of Eq. (1). The corresponding Keldysh kernels are

$$\mathcal{D}_C^R(\omega) = \frac{i}{\hbar} \int_0^\infty dt e^{i\omega t} \langle [F_X^{(C)}(t), F_X^{(C)}(0)] \rangle_C, \quad (\text{B11})$$

$$\mathcal{N}_C(\omega) = \frac{1}{\hbar} \int_{-\infty}^\infty dt e^{i\omega t} \frac{1}{2} \langle \{F_X^{(C)}(t), F_X^{(C)}(0)\} \rangle_C, \quad (\text{B12})$$

where $\langle \dots \rangle_C$ denotes the thermal average for the phonon Hamiltonian $H_{\text{ph}}^{(C)}$ at fixed configuration. These are exactly the force-force expressions of the ordered theory, now with an explicit configuration label and with the Kanzaki field of the disordered alloy.

3. Mode representation of the force

We now expand the force operator $F_X^{(C)}$ in the normal modes of the configuration-dependent harmonic problem. The phonon coordinates can be written as

$$u_i(\mathbf{R}, t; C) = \sum_v \sqrt{\frac{\hbar}{2M_{\text{ref}}\omega_{vC}}} e_i^{(vC)}(\mathbf{R}) (a_{vC}(t) + a_{vC}^\dagger(t)), \quad (\text{B13})$$

with eigenfrequencies ω_{vC} and eigenvectors $e^{(vC)}$ defined in Eq. (A11), and with the usual time evolution

$$a_{vC}(t) = a_{vC} e^{-i\omega_{vC}t}, \quad a_{vC}^\dagger(t) = a_{vC}^\dagger e^{i\omega_{vC}t}. \quad (\text{B14})$$

Inserting Eq. (B13) into Eq. (B10) we obtain

$$F_X^{(C)}(t) = \sum_v C_{vC} Q_{vC}(t), \quad (\text{B15})$$

with mode coordinate

$$Q_{vC}(t) = a_{vC}(t) + a_{vC}^\dagger(t), \quad (\text{B16})$$

and a configuration-dependent slip-phonon vertex

$$C_{vC} = - \sqrt{\frac{\hbar}{2M_{\text{ref}}\omega_{vC}}} \sum_{\mathbf{R}, i} [\partial_X f_i^K(\mathbf{R}; X; C)] e_i^{(vC)}(\mathbf{R}). \quad (\text{B17})$$

This is the disordered analog of the ordered vertex C_λ that appears in Eq. (81): it is the normal-mode projection of the Kanzaki force gradient along the glide coordinate, evaluated on the chosen reference trajectory X .

The oscillator averages at fixed C are standard,

$$\langle a_{vC}^\dagger a_{\mu C} \rangle_C = \delta_{v\mu} n_B(\omega_{vC}), \quad (\text{B18})$$

$$\langle a_{vC} a_{\mu C}^\dagger \rangle_C = \delta_{v\mu} [n_B(\omega_{vC}) + 1], \quad (\text{B19})$$

with $n_B(\omega) = (e^{\beta\hbar\omega} - 1)^{-1}$, and they give the mode correlators

$$\langle [Q_{vC}(t), Q_{\mu C}(0)] \rangle_C = -2i\delta_{v\mu} \sin(\omega_{vC}t), \quad (\text{B20})$$

$$\frac{1}{2} \langle \{Q_{vC}(t), Q_{\mu C}(0)\} \rangle_C = \delta_{v\mu} [2n_B(\omega_{vC}) + 1] \cos(\omega_{vC}t). \quad (\text{B21})$$

Substituting Eqs. (B15) to (B21) into Eqs. (B11) and (B12) yields the configuration-resolved kernels in the time domain,

$$\mathcal{D}_C^R(t) = \theta(t) \frac{1}{\hbar} \sum_v |C_{vC}|^2 \sin(\omega_{vC}t), \quad (\text{B22})$$

$$\mathcal{N}_C(t) = \frac{1}{\hbar} \sum_v |C_{vC}|^2 [2n_B(\omega_{vC}) + 1] \cos(\omega_{vC}t). \quad (\text{B23})$$

The retarded kernel is temperature independent, while the noise kernel carries the full Bose statistics through the factor $2n_B + 1$. No linearization in the sense of a small displacement expansion has been introduced beyond the standard quadratic truncation in the Keldysh action.

4. Spectral representation and relation to mobility kernels

For later use, it is convenient to condense the mode sum in Eq. (B22) into a configuration-resolved spectral density

$$J_C(\Omega) = \frac{\pi}{\hbar} \sum_v |C_{vC}|^2 \delta(\Omega - \omega_{vC}), \quad \Omega > 0. \quad (\text{B24})$$

Using

$$\int_0^\infty dt e^{i\omega t} \sin(\Omega t) = \frac{1}{2} \left[\frac{1}{\omega - \Omega + i0^+} - \frac{1}{\omega + \Omega + i0^+} \right], \quad (\text{B25})$$

the Fourier transform of Eq. (B22) can be written as

$$\mathcal{D}_C^R(\omega) = \int_0^\infty \frac{d\Omega}{\pi} J_C(\Omega) \left[\frac{1}{\omega - \Omega + i0^+} - \frac{1}{\omega + \Omega + i0^+} \right]. \quad (\text{B26})$$

Equivalently, in Laplace space

$$\hat{\mathcal{D}}_C^R(s) = \int_0^\infty dt e^{-st} \mathcal{D}_C^R(t) = \int_0^\infty \frac{d\Omega}{\pi} J_C(\Omega) \frac{s}{s^2 + \Omega^2}, \quad (\text{B27})$$

for $\text{Re } s > 0$. This Stieltjes structure is the direct oscillator analog of the phonon integrals that lead to Eq. (81) in the ordered problem. When the explicit Volterra slip geometry is reinstated, the ordered kernel $\hat{\Gamma}_T^{(n)}(s)$ in Eq. (81) is obtained by inserting, in place of the generic vertex C_λ , the specific slip-phonon vertex

$$C_\lambda = \Phi_{ij}(\mathbf{k}) B_j e_{i,\alpha}(\mathbf{k}) \quad (\text{B28})$$

and summing over branches and Brillouin-zone wave vectors. In the disordered alloy, the configuration-resolved kernel $\hat{\Gamma}_{T,C}^{(n)}(s)$ is constructed in exactly the same way, with the ordered mode data $\{\omega_\lambda, C_\lambda\}$ replaced by $\{\omega_{\nu C}, C_{\nu C}\}$. The high-entropy alloy kernels that enter the mobility law are then defined by configurational averaging of the corresponding spectral densities $J_C(\Omega)$ or, at higher order, of their generalizations $\rho_C^{(n)}(\Omega)$, in direct analogy with the ordered case.

APPENDIX C: TEMPERATURE ASYMPTOTICS OF THE PHONON DRAG COEFFICIENT

This appendix derives the asymptotic temperature dependence of the linear drag coefficient directly from the spectral representation of the mobility kernel. Both the high-temperature and low-temperature limits follow from the same expression and are controlled by the Bose occupation factor together with the infrared structure of the line-projected spectral density.

The static linear drag coefficient at temperature T can be written as

$$B(T) = \int_0^\infty \frac{d\Omega}{\Omega} \rho(\Omega) \coth\left(\frac{\beta\hbar\Omega}{2}\right), \quad (\text{C1})$$

where $\rho(\Omega) \equiv \rho_1^{\text{HEA}}(\Omega)$ is the disorder-averaged line-projected spectral density defined in Sec. II. Separating zero-point and thermal contributions gives

$$B(T) = B_0 + \Delta B(T), \quad B_0 = \int_0^\infty \frac{d\Omega}{\Omega} \rho(\Omega), \quad (\text{C2})$$

$$\Delta B(T) = 2 \int_0^\infty \frac{d\Omega}{\Omega} \rho(\Omega) n_B(\Omega), \quad (\text{C3})$$

with $n_B(\Omega) = (e^{\beta\hbar\Omega} - 1)^{-1}$. All temperature dependence resides in $\Delta B(T)$.

1. High-temperature limit

In the classical regime $k_B T \gg \hbar\Omega$, the Bose factor admits the expansion

$$n_B(\Omega) \simeq \frac{k_B T}{\hbar\Omega}. \quad (\text{C4})$$

Substitution into Eq. (C3) yields

$$\Delta B(T) \simeq \frac{2k_B T}{\hbar} \int_0^\infty d\Omega \frac{\rho(\Omega)}{\Omega^2}, \quad (\text{C5})$$

provided the integral converges. The drag coefficient therefore obeys

$$B(T) = B_0 + B' T, \quad (\text{C6})$$

with

$$B' = \frac{2k_B}{\hbar} \int_0^\infty d\Omega \frac{\rho(\Omega)}{\Omega^2}. \quad (\text{C7})$$

This linear scaling is a direct consequence of classical equipartition and does not depend on the detailed low-frequency behavior of $\rho(\Omega)$.

2. Low-temperature limit

In the quantum regime $k_B T \ll \hbar\Omega_D$, thermal occupation is restricted to long-wavelength phonons. The temperature dependence of the drag is therefore controlled entirely by the infrared structure of the line-projected spectral density $\rho(\Omega)$. No assumption on its form is required *a priori*; instead, its low-frequency behavior follows from general constraints on the Kanzaki coupling and the acoustic-phonon spectrum.

For a stable three-dimensional crystal, acoustic-phonon branches satisfy $\omega_\lambda(\mathbf{q}) \sim c_\lambda |\mathbf{q}|$ as $|\mathbf{q}| \rightarrow 0$, and the phonon density of states scales as Ω^2 . The Kanzaki force represents a force dipole distribution associated with the dislocation core. Mechanical equilibrium requires the net force exerted by the Kanzaki field on the lattice to vanish, which removes monopole contributions and implies that the Kanzaki vertex vanishes linearly with wave vector for long-wavelength modes. As a consequence, the squared coupling entering the spectral density scales at least as $|g_\nu|^2 \propto |\mathbf{q}|^2$ for acoustic phonons.

We therefore specialize to the linear kernel, so $n = 1$ and we write $\rho(\Omega) \equiv \rho_1(\Omega)$. In the Bloch limit, the mode index ν becomes $(\lambda, \mathbf{q})$, with acoustic branches $\lambda \in \{1, 2, 3\}$ and $\mathbf{q}$ in the first Brillouin zone. Equation (23) reduces, up to conventions already fixed in the main text, to a Brillouin-zone integral of the form

$$\rho(\Omega) = \frac{\hbar}{\varrho} \sum_\lambda \int_{\text{BZ}} \frac{d^3 q}{(2\pi)^3} \frac{|q_\parallel|}{\omega_\lambda(\mathbf{q})} |C_\lambda(\mathbf{q})|^2 \delta(\Omega - \omega_\lambda(\mathbf{q})), \quad (\text{C8})$$

where $q_\parallel = \mathbf{q} \cdot \hat{\mathbf{z}}$ is the component along the dislocation line, and $C_\lambda(\mathbf{q})$ is the line-projected vertex defined in Eq. (22) in the Bloch basis. The low-frequency asymptotics follow from the neighborhood of $\mathbf{q} = \mathbf{0}$.

For acoustic branches, stability implies a linear dispersion:

$$\omega_\lambda(\mathbf{q}) = c_\lambda(\hat{\mathbf{q}}) |\mathbf{q}| + o(|\mathbf{q}|), \quad |\mathbf{q}| \rightarrow 0, \quad (\text{C9})$$

with direction-dependent sound speed $c_\lambda(\hat{\mathbf{q}})$. Substituting Eq. (C9) into Eq. (C8) and restricting the integral to a small ball $|\mathbf{q}| < q_0$, one may write $\mathbf{q} = q\hat{\mathbf{q}}$ and use $d^3 q = q^2 dq d\Omega_{\hat{\mathbf{q}}}$ to obtain

$$\begin{aligned} \rho(\Omega) &\simeq \frac{\hbar}{\varrho} \sum_\lambda \int d\Omega_{\hat{\mathbf{q}}} \int_0^{q_0} \frac{q^2 dq}{(2\pi)^3} \frac{q |\hat{\mathbf{q}} \cdot \hat{\mathbf{z}}|}{c_\lambda(\hat{\mathbf{q}}) q} \\ &\times |C_\lambda(q\hat{\mathbf{q}})|^2 \delta(\Omega - c_\lambda(\hat{\mathbf{q}}) q). \end{aligned} \quad (\text{C10})$$

The factor $q |\hat{\mathbf{q}} \cdot \hat{\mathbf{z}}|$ comes from $|q_\parallel|$. The factor $1/\omega_\lambda$ contributes $1/(c_\lambda q)$.

The radial integral is evaluated by the delta function. Using

$$\delta(\Omega - c_\lambda(\hat{\mathbf{q}}) q) = \frac{1}{c_\lambda(\hat{\mathbf{q}})} \delta\left(q - \frac{\Omega}{c_\lambda(\hat{\mathbf{q}})}\right), \quad (\text{C11})$$

Eq. (C10) becomes

$$\rho(\Omega) \simeq \frac{\hbar}{\varrho} \sum_{\lambda} \int d\Omega_{\mathbf{q}} \frac{1}{(2\pi)^3} \frac{\Omega^2}{c_{\lambda}(\mathbf{q})^3} \frac{\Omega |\hat{\mathbf{q}} \cdot \hat{\mathbf{z}}|}{c_{\lambda}(\mathbf{q})} \left| C_{\lambda} \left(\frac{\Omega}{c_{\lambda}(\mathbf{q})} \hat{\mathbf{q}} \right) \right|^2. \quad (\text{C12})$$

At this point, the entire question reduces to the infrared scaling of the vertex $C_{\lambda}(\mathbf{q})$.

To extract that scaling, return to Eq. (22). In an ordered crystal, the eigenvector is a plane wave, and the sum over $\mathbf{R}$ produces the Fourier transform of the driving field $\partial_X f^K$ evaluated at $\mathbf{q}$. More precisely, one obtains

$$C_{\lambda}(\mathbf{q}) = \sqrt{\frac{\hbar}{2M_{\text{ref}}\omega_{\lambda}(\mathbf{q})}} \mathbf{e}_{\lambda}(\hat{\mathbf{q}}) \cdot \mathbf{F}(\mathbf{q}), \quad (\text{C13})$$

where $\mathbf{e}_{\lambda}$ is the acoustic polarization vector and

$$\mathbf{F}(\mathbf{q}) = \sum_{\mathbf{R}} \partial_X \mathbf{f}^K(\mathbf{R}) e^{-i\mathbf{q} \cdot \mathbf{R}} \quad (\text{C14})$$

is the discrete Fourier transform of the driving field. The crucial structural constraint is the mechanical equilibrium of the static Kanzaki source itself. Let $\mathbf{f}^K(\mathbf{R})$ denote the force distribution associated with a straight dislocation at a fixed position. Mechanical equilibrium of the defect implies

$$\sum_{\mathbf{R}} \mathbf{f}^K(\mathbf{R}) = \mathbf{0}, \quad (\text{C15})$$

so that its Fourier transform satisfies

$$\mathbf{f}^K(\mathbf{q}) = \sum_{\mathbf{R}} \mathbf{f}^K(\mathbf{R}) e^{-i\mathbf{q} \cdot \mathbf{R}} = O(|\mathbf{q}|), \quad |\mathbf{q}| \rightarrow 0. \quad (\text{C16})$$

In the phonon-wind problem, the relevant driving field is not an arbitrary localized force distribution but the change of the static Kanzaki source under an infinitesimal rigid translation of the dislocation. A translation along the glide direction x yields

$$\partial_X \mathbf{f}^K(\mathbf{R}) = -\partial_X \mathbf{f}^K(\mathbf{R}), \quad (\text{C17})$$

and, therefore, in Fourier space,

$$\mathbf{F}(\mathbf{q}) = \sum_{\mathbf{R}} \partial_X \mathbf{f}^K(\mathbf{R}) e^{-i\mathbf{q} \cdot \mathbf{R}} = i q_X \mathbf{f}^K(\mathbf{q}). \quad (\text{C18})$$

Combining Eqs. (C16) and (C18) gives the infrared behavior

$$\mathbf{F}(\mathbf{q}) = O(|\mathbf{q}|^2), \quad |\mathbf{q}| \rightarrow 0. \quad (\text{C19})$$

Thus, the leading coupling of long-wavelength acoustic phonons to a rigidly translated, force-balanced dislocation is quadrupolar rather than dipolar.

Substituting Eq. (C19) into Eq. (C13) and using $\omega_{\lambda}(\mathbf{q}) \sim c_{\lambda} |\mathbf{q}|$ yields

$$|C_{\lambda}(\mathbf{q})|^2 \sim \frac{\hbar}{2M_{\text{ref}}} \frac{|\mathbf{F}(\mathbf{q})|^2}{\omega_{\lambda}(\mathbf{q})} \propto \frac{|\mathbf{q}|^4}{|\mathbf{q}|} \propto |\mathbf{q}|^3, \quad |\mathbf{q}| \rightarrow 0. \quad (\text{C20})$$

Since the phase-space and kinematic prefactors in Eq. (C8) contribute Ω^2 for acoustic modes, substituting $|\mathbf{q}| \sim \Omega/c_{\lambda}$ into Eq. (C20) gives

$$\rho(\Omega) \propto \Omega^5, \quad \Omega \rightarrow 0. \quad (\text{C21})$$

The low-temperature correction therefore obeys

$$\Delta B(T) \propto T^5. \quad (\text{C22})$$

3. Physical implications

For a rigidly translated straight dislocation whose static Kanzaki source is force balanced, the infrared structure of the coupling is quadrupolar, leading to $\rho(\Omega) \propto \Omega^5$ and hence

$$\Delta B(T) \propto T^5. \quad (\text{C23})$$

This reproduces the classical low-temperature phonon wind scaling reported in the Leibfried–Alshits tradition [81,137] and in subsequent treatments based on rigid transport of the long-range elastic field.

We note that a T^3 law arises if one considers a generic dipolar coupling satisfying only force neutrality of the driving field $\partial_X f^K$ without enforcing its origin as the translation derivative of a force-balanced static source. In that case $|\mathbf{F}(\mathbf{q})| = O(|\mathbf{q}|)$ and the spectral density scales as $\rho(\Omega) \propto \Omega^3$. The exponent therefore provides a diagnostic of whether the infrared coupling is effectively dipolar or quadrupolar.

- [1] B. Cantor, I. T. H. Chang, P. Knight, and A. J. B. Vincent, Microstructural development in equiatomic multicomponent alloys, *Mater. Sci. Eng. A* **375-377**, 213 (2004).
- [2] J.-W. Yeh, S.-K. Chen, S.-J. Lin, J.-Y. Gan, T.-S. Chin, T.-T. Shun, C.-H. Tsau, and S.-Y. Chang, Nanostructured high-entropy alloys with multiple principal elements: Novel alloy design concepts and outcomes, *Adv. Eng. Mater.* **6**, 299 (2004).
- [3] E. P. George, D. Raabe, and R. O. Ritchie, High-entropy alloys, *Nat. Rev. Mater.* **4**, 515 (2019).
- [4] D. B. Miracle and O. N. Senkov, A critical review of high entropy alloys and related concepts, *Acta Mater.* **122**, 448 (2017).
- [5] O. N. Senkov, G. B. Wilks, J. M. Scott, and D. B. Miracle, Mechanical properties of $\text{Nb}_{25}\text{Mo}_{25}\text{Ta}_{25}\text{W}_{25}$

and $\text{v}_{20}\text{Nb}_{20}\text{Mo}_{20}\text{Ta}_{20}\text{W}_{20}$ refractory high entropy alloys, *Intermetallics* **19**, 698 (2011).

- [6] K.-Y. Wang, Z.-J. Cheng, Z.-L. Ning, H.-P. Yu, P. Ramasamy, J. Eckert, J.-F. Sun, A. H. W. Ngan, and Y.-J. Huang, Unraveling the cryogenic formability in high entropy alloy sheets under complex stress conditions, *Rare Met.* **44**, 1332 (2025).
- [7] S. Wang, M. Wu, D. Shu, G. Zhu, D. Wang, and B. Sun, Mechanical instability and tensile properties of TiZrHfNbTa high entropy alloy at cryogenic temperatures, *Acta Mater.* **201**, 517 (2020).
- [8] J. P. Hirth and J. Lothe, *Theory of Dislocations*, 2nd ed. (John Wiley & Sons, New York, 1982).
- [9] A. P. Sutton, *Physics of Elasticity and Crystal Defects* (Oxford University Press, Oxford, UK, 2024), Vol. 6.

- [10] V. Vitek and V. Paidar, Non-planar dislocation cores: A ubiquitous phenomenon affecting mechanical properties of crystalline materials, in *Dislocations in Solids* (Elsevier, London, UK, 2008), Vol. 14, pp. 439–514.
- [11] W. P. Mason, Phonon viscosity and its effect on acoustic wave attenuation and dislocation motion, *J. Acoust. Soc. Am.* **32**, 458 (1960).
- [12] V. I. Alshits, Phononnyj veter i tormozhenije dislokaczij, *Fiz. Tvier. Tiela* **11**, 2405 (1969).
- [13] V. I. Alshits, *The phonon-dislocation interaction and its Role in Dislocation Dragging and Thermal Resistivity* (Elsevier, London, UK, 1992), Vol. 31, pp. 625–697.
- [14] J. D. Eshelby, Uniformly moving dislocations, *Proc. Phys. Soc. London, Sect. A* **62**, 307 (1949).
- [15] D. N. Blaschke, Properties of dislocation drag from phonon wind at ambient conditions, *Materials* **12**, 948 (2019).
- [16] P. Gumbsch and H. Gao, Dislocations faster than the speed of sound, *Science* **283**, 965 (1999).
- [17] D. L. Olmsted, L. G. Hector Jr, W. A. Curtin, and R. J. Clifton, Atomistic simulations of dislocation mobility in Al, Ni and Al/Mg alloys, *Modell. Simul. Mater. Sci. Eng.* **13**, 371 (2005).
- [18] M. R. Gilbert, S. Queyreau, and J. Marian, Stress and temperature dependence of screw dislocation mobility in α -Fe by molecular dynamics, *Phys. Rev. B* **84**, 174103 (2011).
- [19] W. G. Johnston and J. J. Gilman, Dislocation velocities, dislocation densities, and plastic flow in lithium fluoride crystals, *J. Appl. Phys.* **30**, 129 (1959).
- [20] T. Vreeland Jr. and K. M. Jassby, Dislocation-phonon interactions and dynamic behaviour of individual dislocations as observed by stress pulse method, *Cryst. Lattice Defects* **4**, 1 (1973).
- [21] L. R. Owen, N. G. Jones, Lattice distortions in high-entropy alloys, *J. Mater. Res.* **33**, 2954 (2018).
- [22] W. Li, S. Lyu, Y. Chen, and A. H. W. Ngan, Fluctuations in local shear-fault energy produce unique and dominating strengthening in metastable complex concentrated alloys, *Proc. Natl. Acad. Sci. USA* **120**, e2209188120 (2023).
- [23] Y. Hu, L. R. Owen, H. Y. Playford, A. Edgren, S. Guo, and M. H. Colliander, Quantifying local lattice distortions in refractory high-entropy alloys, *Phys. Rev. Mater.* **8**, 083602 (2024).
- [24] F. Körmann, Y. Ikeda, B. Grabowski, and M. H. F. Sluiter, Phonon broadening in high entropy alloys, *npj Comput. Mater.* **3**, 36 (2017).
- [25] G. Ek, Ø. S. Fjellvåg, P. Vajeeston, J. Armstrong, M. Sahlberg, and U. Häussermann, Vibrational properties of high entropy alloy based metal hydrides probed by inelastic neutron scattering, *J. Alloys Compd.* **877**, 160320 (2021).
- [26] A. Haglund, M. Koehler, D. Catoor, E. P. George, and V. Keppens, Polycrystalline elastic moduli of a high-entropy alloy at cryogenic temperatures, *Intermetallics* **58**, 62 (2015).
- [27] L. R. Owen, E. J. Pickering, H. Y. Playford, H. J. Stone, M. G. Tucker, and N. G. Jones, An assessment of the lattice strain in the CrMnFeCoNi high-entropy alloy, *Acta Mater.* **122**, 11 (2017).
- [28] Y. Cao, K. Sheriff, and R. Freitas, Capturing short-range order in high-entropy alloys with machine learning potentials, *npj Comput. Mater.* **11**, 268 (2025).
- [29] A. V. Shapeev, Moment tensor potentials: A class of systematically improvable interatomic potentials, *Multisc. Model. Simul.* **14**, 1153 (2016).
- [30] S. Yin, Y. Zuo, A. Abu-Odeh, H. Zheng, X.-G. Li, J. Ding, S. P. Ong, M. Asta, and R. O. Ritchie, Atomistic simulations of dislocation mobility in refractory high-entropy alloys and the effect of chemical short-range order, *Nat. Commun.* **12**, 4873 (2021).
- [31] D. Utt, S. Lee, Y. Xing, H. Jeong, A. Stukowski, S. H. Oh, G. Dehm, and K. Albe, The origin of jerky dislocation motion in high-entropy alloys, *Nat. Commun.* **13**, 4777 (2022).
- [32] M. R. Jones, P. Garg, and I. J. Beyerlein, Transitions in thermally activated glide mechanisms in the MoNbTaVW refractory multiprincipal element alloy up to 0.3 t_m , *Phys. Rev. Mater.* **8**, 103603 (2024).
- [33] R. Pasianot and D. Farkas, Atomistic modeling of dislocations in a random quinary high-entropy alloy, *Comput. Mater. Sci.* **173**, 109366 (2020).
- [34] S. Lyu, Y. Xia, W. Li, T. Zhu, Y. Chen, and A. H. W. Ngan, Statistical mechanics, entropy and temperature analog of dislocations moving on fluctuating resistance landscapes, *Acta Mater.* **291**, 121002 (2025).
- [35] R. B. Sills, M. E. Foster, and X. W. Zhou, Line-length-dependent dislocation mobilities in an fcc stainless steel alloy, *Int. J. Plast.* **135**, 102791 (2020).
- [36] K. Chu, M. E. Foster, R. B. Sills, X. Zhou, T. Zhu, and D. L. McDowell, Temperature and composition dependent screw dislocation mobility in austenitic stainless steels from large-scale molecular dynamics, *npj Comput. Mater.* **6**, 179 (2020).
- [37] X. Zhou, S. He, and J. Marian, Cross-kinks control screw dislocation strength in equiatomic bcc refractory alloys, *Acta Mater.* **211**, 116875 (2021).
- [38] L. Romaner, C. Ambrosch-Draxl, and R. Pippan, Effect of rhenium on the dislocation core structure in tungsten, *Phys. Rev. Lett.* **104**, 195503 (2010).
- [39] F. Maresca and W. A. Curtin, Mechanistic origin of high strength in refractory bcc high entropy alloys up to 1900K, *Acta Mater.* **182**, 235 (2020).
- [40] S. I. Rao, C. Varvenne, C. Woodward, T. A. Parthasarathy, D. Miracle, O. N. Senkov, and W. A. Curtin, Atomistic simulations of dislocations in a model bcc multicomponent concentrated solid solution alloy, *Acta Mater.* **125**, 311 (2017).
- [41] F. Körmann, A. V. Ruban, and M. H. F. Sluiter, Long-ranged interactions in bcc NbMoTaW high-entropy alloys, *Mater. Res. Lett.* **5**, 35 (2017).
- [42] S. I. Rao, B. Akdim, E. Antillon, C. Woodward, T. A. Parthasarathy, and O. N. Senkov, Modeling solution hardening in bcc refractory complex concentrated alloys: NbTiZr, Nb_{1.5}TiZr_{0.5} and Nb_{0.5}TiZr_{1.5}, *Acta Mater.* **168**, 222 (2019).
- [43] X. Liu, T. P. Moran, B. F. G. Aymon, and W. A. Curtin, Peierls-Nabarro modeling of dislocations in high-entropy alloys, *J. Mech. Phys. Solids* **208**, 106457 (2025).
- [44] F. Tian, A review of solid-solution models of high-entropy alloys based on *ab initio* calculations, *Front. Mater.* **4**, 36 (2017).
- [45] P. Soven, Coherent-potential model of substitutional disordered alloys, *Phys. Rev.* **156**, 809 (1967).
- [46] J. Korringa, On the calculation of the energy of a Bloch wave in a metal, *Physica* **13**, 392 (1947).

- [47] W. Kohn and N. Rostoker, Solution of the Schrödinger equation in periodic lattices with an application to metallic lithium, *Phys. Rev.* **94**, 1111 (1954).
- [48] B. L. Gyorffy, Coherent-potential approximation for a nonoverlapping-muffin-tin-potential model of random substitutional alloys, *Phys. Rev. B* **5**, 2382 (1972).
- [49] L. Vitos, *Computational Quantum Mechanics for Materials Engineers: The EMTO Method and Applications* (Springer, New York, 2007).
- [50] H. Ebert, D. Koedderitzsch, and J. Minar, Calculating condensed matter properties using the KKR-Green's function method—recent developments and applications, *Rep. Prog. Phys.* **74**, 096501 (2011).
- [51] F. Tian, L. K. Varga, J. Shen, and L. Vitos, Calculating elastic constants in high-entropy alloys using the coherent potential approximation: Current issues and errors, *Comput. Mater. Sci.* **111**, 350 (2016).
- [52] S. Huang, W. Li, S. Lu, F. Tian, J. Shen, E. Holmström, and L. Vitos, Temperature dependent stacking fault energy of FeCrCoNiMn high entropy alloy, *Scr. Mater.* **108**, 44 (2015).
- [53] S. Ghosh, P. L. Leath, and M. H. Cohen, Phonons in random alloys: The itinerant coherent-potential approximation, *Phys. Rev. B* **66**, 214206 (2002).
- [54] Y. Ikeda, F. Körmann, B. Dutta, A. Carreras, A. Seko, J. Neugebauer, and I. Tanaka, Temperature-dependent phonon spectra of magnetic random solid solutions, *npj Comput. Mater.* **4**, 7 (2018).
- [55] W. R. Mondal, N. S. Vidhyadhiraja, T. Berlijn, J. Moreno, and M. Jarrell, Localization of phonons in mass-disordered alloys: A typical medium dynamical cluster approach, *Phys. Rev. B* **96**, 014203 (2017).
- [56] W. R. Mondal, T. Berlijn, M. Jarrell, and N. S. Vidhyadhiraja, Phonon localization in binary alloys with diagonal and off-diagonal disorder: A cluster Green's function approach, *Phys. Rev. B* **99**, 134203 (2019).
- [57] W. R. Mondal and N. S. Vidhyadhiraja, Effect of short-ranged spatial correlations on the Anderson localization of phonons in mass-disordered systems, *Bull. Mater. Sci.* **43**, 314 (2020).
- [58] W. R. Mondal, T. Berlijn, N. S. Vidhyadhiraja, and H. Terletska, Typical medium cluster approach for multibranch phonon localization, *Phys. Rev. B* **113**, 064203 (2026).
- [59] A. Zunger, S.-H. Wei, L. G. Ferreira, and J. E. Bernard, Special quasirandom structures, *Phys. Rev. Lett.* **65**, 353 (1990).
- [60] L.-Y. Tian, Q.-M. Hu, R. Yang, J. Zhao, B. Johansson, and L. Vitos, Elastic constants of random solid solutions by SQS and CPA approaches: The case of fcc Ti-Al, *J. Phys.: Condens. Matter* **27**, 315702 (2015).
- [61] L.-Y. Tian, L.-H. Ye, Q.-M. Hu, S. Lu, J. Zhao, and L. Vitos, CPA descriptions of random Cu-Au alloys in comparison with SQS approach, *Comput. Mater. Sci.* **128**, 302 (2017).
- [62] M. Karabin, W. R. Mondal, A. Östlin, W.-G. D. Ho, V. Dobrosavljevic, K.-M. Tam, H. Terletska, L. Chioncel, Y. Wang, and M. Eisenbach, *Ab initio* approaches to high-entropy alloys: A comparison of CPA, SQS, and supercell methods, *J. Mater. Sci.* **57**, 10677 (2022).
- [63] C. Varvenne, G. P. M. Leyson, M. Ghazisaeidi, and W. A. Curtin, Solute strengthening in random alloys, *Acta Mater.* **124**, 660 (2017).
- [64] C. Varvenne, A. Luque, and W. A. Curtin, Theory of strengthening in fcc high entropy alloys, *Acta Mater.* **118**, 164 (2016).
- [65] F. Maresca and W. A. Curtin, Theory of screw dislocation strengthening in random bcc alloys from dilute to “high-entropy” alloys, *Acta Mater.* **182**, 144 (2020).
- [66] R. Labusch, A statistical theory of solid solution hardening, *Phys. Status Solidi B* **41**, 659 (1970).
- [67] G. Laplanche, A. Kostka, C. Reinhart, J. Hunfeld, G. Eggeler, and E. P. George, Reasons for the superior mechanical properties of medium-entropy CrCoNi compared to high-entropy CrMnFeCoNi, *Acta Mater.* **128**, 292 (2017).
- [68] G. Bracq, M. Laurent-Brocq, C. Varvenne, L. Perrière, W. A. Curtin, J.-M. Joubert, and I. Guillot, Combining experiments and modeling to explore the solid solution strengthening of high and medium entropy alloys, *Acta Mater.* **177**, 266 (2019).
- [69] C. Lee, F. Maresca, R. Feng, Y. Chou, T. Ungar, M. Widom, K. An, J. D. Poplawsky, Y.-C. Chou, P. K. Liaw, *et al.*, Strength can be controlled by edge dislocations in refractory high-entropy alloys, *Nat. Commun.* **12**, 5474 (2021).
- [70] R. E. Kubilay, A. Ghafarollahi, F. Maresca, and W. A. Curtin, High energy barriers for edge dislocation motion in body-centered cubic high entropy alloys, *npj Comput. Mater.* **7**, 112 (2021).
- [71] B. Gurrutxaga-Lerma, Quantum statistical theory of dislocation mobility in discrete lattices, *Phys. Rev. Mater.* **9**, 123605 (2025).
- [72] I. Batatia, D. P. Kovacs, G. Simm, C. Ortner, and G. Csányi, MACE: Higher order equivariant message passing neural networks for fast and accurate force fields, in *Advances in Neural Information Processing Systems*, edited by S. Koyejo, S. Mohamed, A. Agarwal, D. Belgrave, K. Cho, and A. Oh (Curran Associates, 2022), Vol. 35, pp. 11423–11436.
- [73] H. Kanzaki, Point defects in face-centred cubic lattice—I distortion around defects, *J. Phys. Chem. Solids* **2**, 24 (1957).
- [74] H. Kanzaki, Point defects in face-centred cubic lattice—II X-ray scattering effects, *J. Phys. Chem. Solids* **2**, 107 (1957).
- [75] B. Gurrutxaga-Lerma and J. Verschuereen, Elastic models of dislocations based on atomistic Kanzaki forces, *Phys. Rev. B* **98**, 134104 (2018).
- [76] B. Gurrutxaga-Lerma and J. Verschuereen, Generalized Kanzaki force field of extended defects in crystals with applications to the modeling of edge dislocations, *Phys. Rev. Mater.* **3**, 113801 (2019).
- [77] R. P. Feynman and F. L. Vernon Jr., The theory of a general quantum system interacting with a linear dissipative system, *Ann. Phys. (NY)* **281**, 547 (2000).
- [78] L. V. Keldysh, Diagram technique for nonequilibrium processes, in *Selected Papers of Leonid V. Keldysh* (World Scientific, Singapore, 2024), pp. 47–55.
- [79] A. Kamenev, *Field Theory of Non-Equilibrium Systems* (Cambridge University Press, Cambridge, 2023).
- [80] U. Weiss, *Quantum Dissipative Systems*, 4th ed. (World Scientific, Singapore, 2012).
- [81] G. Leibfried, Über den Einfluß thermisch angeregter Schallwellen auf die plastische Deformation, *Eur. Phys. J. A* **127**, 344 (1950).
- [82] B. Gurrutxaga-Lerma, *Ab initio* theory of electron drag and wind forces on dislocations: Bridging quantum transport and electroplasticity, *Phys. Rev. Mater.* **10**, 033803 (2026).
- [83] R. L. Schilling, R. Song, and Z. Vondracek, *Bernstein Functions: Theory and Applications* (Walter de Gruyter, 2012), Vol. 37.

- [84] M. Mézard, G. Parisi, and M. A. Virasoro, Spin glass theory and beyond, *World Scientific Lecture Notes in Physics*, Vol. 9 (World Scientific, New York, 1986).
- [85] M. Kardar, *Statistical Physics of Fields* (Cambridge University Press, Cambridge, 2007).
- [86] F. Yonezawa and K. Morigaki, Coherent potential approximation. Basic concepts and applications, *Prog. Theor. Phys. Suppl.* **53**, 1 (1973).
- [87] H. Nishimori, *Statistical Physics of Spin Glasses and Information Processing: An Introduction, Number 111* (Clarendon Press, 2001).
- [88] A. Alam, R. K. Chouhan, and A. Mookerjee, Phonon modes and vibrational entropy of disordered alloys with short-range order: A first-principles calculation, *Phys. Rev. B* **83**, 054201 (2011).
- [89] D. R. Trinkle, Lattice Green function for extended defect calculations: Computation and error estimation with long-range forces, *Phys. Rev. B* **78**, 014110 (2008).
- [90] J. E. Sinclair, P. C. Gehlen, R. G. Hoagland, and J. P. Hirth, Flexible boundary conditions and nonlinear geometric effects in atomic dislocation modeling, *J. Appl. Phys.* **49**, 3890 (1978).
- [91] G. H. Golub and C. F. Van Loan, *Matrix Computations* (John Hopkins University Press, 2013).
- [92] Z. Huang, E. Gull, and L. Lin, Robust analytic continuation of Green's functions via projection, pole estimation, and semidefinite relaxation, *Phys. Rev. B* **107**, 075151 (2023).
- [93] A. Luger and M.-J. Yvonne Ou, On applications of Herglotz-Nevanlinna functions in material sciences, I: Classical theory and applications of sum rules, in *Research in Mathematics of Materials Science* (Springer, Berlin, 2022), pp. 433–459.
- [94] S. R. Turner, S. Pailhès, F. Bourdarot, J. Ollivier, Y. Sidis, J.-P. Castellan, J.-M. Zanotti, Q. Berrod, F. Porcher, A. Bosak, *et al.*, Phonon behavior in a random solid solution: A lattice dynamics study on the high-entropy alloy FeCoCrMnNi, *Nat. Commun.* **13**, 7509 (2022).
- [95] M. Born and K. Huang, *Dynamical Theory of Crystal Lattices* (Oxford University Press, New York, 1998).
- [96] A. Togo and I. Tanaka, First principles phonon calculations in materials science, *Scr. Mater.* **108**, 1 (2015).
- [97] S.-H. Wei and A. Zunger, Disorder effects on the density of states of the II-VI semiconductor alloys $\text{Hg}_{0.5}\text{Cd}_{0.5}\text{Te}$, $\text{Cd}_{0.5}\text{Zn}_{0.5}\text{Te}$, and $\text{Hg}_{0.5}\text{Zn}_{0.5}\text{Te}$, *Phys. Rev. B* **43**, 1662 (1991).
- [98] C. Lin, S. Poncé, and N. Marzari, General invariance and equilibrium conditions for lattice dynamics in 1d, 2d, and 3d materials, *npj Comput. Mater.* **8**, 236 (2022).
- [99] G. J. Ackland, M. C. Warren, and S. J. Clark, Practical methods in *ab initio* lattice dynamics, *J. Phys.: Condens. Matter* **9**, 7861 (1997).
- [100] X. Li, Efficient boundary conditions for molecular statics models of solids, *Phys. Rev. B* **80**, 104112 (2009).
- [101] A. M. Z. Tan, and D. R. Trinkle, Computation of the lattice Green function for a dislocation, *Phys. Rev. E* **94**, 023308 (2016).
- [102] E. N. Economou, *Green's Functions in Quantum Physics* (Springer, Berlin, 2006).
- [103] M. P. LopezSancho, J. M. Lopez Sancho, and J. Rubio, Highly convergent schemes for the calculation of bulk and surface Green functions, *J. Phys. F: Met. Phys.* **15**, 851 (1985).
- [104] B. Gustavsen and A. Semlyen, Rational approximation of frequency domain responses by vector fitting, *IEEE Trans. Power Delivery* **14**, 1052 (2002).
- [105] K. Schmüdgen *et al.*, *The Moment Problem* (Springer, 2017), Vol. 9.
- [106] A. C. Antoulas, *Approximation of Large-Scale Dynamical System* (SIAM, New York, 2005).
- [107] I. P. Cornfeld, S. V. Fomin, and Y. G. Sinai, *Ergodic Theory* (Springer Science & Business Media, 2012).
- [108] X. W. Zhou, R. A. Johnson, and H. N. G. Wadley, Misfit-energy-increasing dislocations in vapor-deposited CoFe/NiFe multilayers, *Phys. Rev. B* **69**, 144113 (2004).
- [109] D. Farkas and A. Caro, Model interatomic potentials and lattice strain in a high-entropy alloy, *J. Mater. Res.* **33**, 3218 (2018).
- [110] J. E. Arnold, C. D. Woodgate, R. Hafizi, M. J. Harris, A. Mottura, G. F. García, and B. Gurrutxaga-Lerma, Thermodynamics and phase stability of the AlTiCrMoW high-entropy alloy simulated using machine-learned interatomic potentials, *Phys. Rev. Mater.* **10**, 073605 (2026).
- [111] S. Queyreau, J. Marian, M. R. Gilbert, and B. D. Wirth, Edge dislocation mobilities in bcc Fe obtained by molecular dynamics, *Phys. Rev. B* **84**, 064106 (2011).
- [112] G. Po, Y. Cui, D. Rivera, D. Cereceda, T. D. Swinburne, J. Marian, and N. Ghoniem, A phenomenological dislocation mobility law for bcc metals, *Acta Mater.* **119**, 123 (2016).
- [113] H. Tsuzuki, P. S. Branicio, and J. P. Rino, Accelerating dislocations to transonic and supersonic speeds in anisotropic metals, *Appl. Phys. Lett.* **92**, 191909 (2008).
- [114] J. Marian and A. Caro, Moving dislocations in disordered alloys: Connecting continuum and discrete models with atomistic simulations, *Phys. Rev. B* **74**, 024113 (2006).
- [115] E. V. der Giessen and A. Needleman, Discrete dislocation plasticity: A simple planar model, *Modell. Simul. Mater. Sci. Eng.* **3**, 689 (1995).
- [116] V. V. Bulatov and W. Cai, *Computer Simulations of Dislocation* (Oxford University Press, Oxford, 2006).
- [117] T. Duong and M. J. Demkowicz, Resonance with surface waves induces forbidden velocity bands in dislocation glide, *J. Mech. Phys. Solids* **180**, 105422 (2023).
- [118] M. H. Müser, S. V. Sukhomlinov, and L. Pastewka, Interatomic potentials: Achievements and challenges, *Adv. Phys.: X* **8**, 2093129 (2023).
- [119] A. Rohskopf, H. R. Seyf, K. Gordiz, T. Tadano, and A. Henry, Empirical interatomic potentials optimized for phonon properties, *npj Comput. Mater.* **3**, 27 (2017).
- [120] R. W. Armstrong, W. Arnold, and F. J. Zerilli, Dislocation mechanics of shock-induced plasticity, *Metall. Mater. Trans. A* **38**, 2605 (2007).
- [121] G. I. Kanel, S. V. Razorenov, E. B. Zaretsky, B. Herrman, and L. Meyer, Thermal “softening” and “hardening” of titanium and its alloy at high strain rates of shock-wave deforming, *Phys. Solid State* **45**, 656 (2003).
- [122] E. B. Zaretsky, Shock response of iron between 143 and 1275 K, *J. Appl. Phys.* **106**, 023510 (2009).
- [123] E. B. Zaretsky and G. I. Kanel, Tantalum and vanadium response to shock-wave loading at normal and elevated temperatures. Non-monotonous decay of the elastic wave in vanadium, *J. Appl. Phys.* **115**, 243502 (2014).

- [124] E. B. Zaretsky, Impact response of cobalt over the 300–1400 K temperature range, *J. Appl. Phys.* **108**, 083525 (2010).
- [125] E. B. Zaretsky and G. I. Kanel, Response of copper to shock-wave loading at temperatures up to the melting point, *J. Appl. Phys.* **114**, 083511 (2013).
- [126] Y. Tang, and D. Y. Li, Dynamic response of high-entropy alloys to ballistic impact, *Sci. Adv.* **8**, eabp9096 (2022).
- [127] G. Laplanche, A. Kostka, O. M. Horst, G. Eggeler, and E. P. George, Microstructure evolution and critical stress for twinning in the CrMnFeCoNi high-entropy alloy, *Acta Mater.* **118**, 152 (2016).
- [128] M. Komarasamy, K. Alagarsamy, and R. S. Mishra, Serration behavior and negative strain rate sensitivity of Al_{0.1}CoCrFeNi high entropy alloy, *Intermetallics* **84**, 20 (2017).
- [129] R. Sonkusare, R. Jain, K. Biswas, V. Parameswaran, and N. P. Gurao, High strain rate compression behaviour of single phase CoCuFeMnNi high entropy alloy, *J. Alloys Compd.* **823**, 153763 (2020).
- [130] Z. Li, S. Zhao, H. Diao, P. K. Liaw, and M. A. Meyers, High-velocity deformation of Al_{0.3}CoCrFeNi high-entropy alloy: Remarkable resistance to shear failure, *Sci. Rep.* **7**, 42742 (2017).
- [131] K. Ren, H. Liu, R. Ma, S. Chen, S. Zhang, R. Wang, R. Chen, Y. Tang, S. Li, and F. Lu, Dynamic compression behavior of TiZrNbV refractory high-entropy alloys upon ultrahigh strain rate loading, *J. Mater. Sci. Technol.* **161**, 201 (2023).
- [132] Y. Xiao, Q. Zeng, K. Xun, J. Ding, L. Wang, L. Wang, Y. Liang, K. Jin, S. Zhu, Y. Ren, *et al.*, Novel mechanism of ultra-high adiabatic shear susceptibility in fcc-based high-entropy alloys via high-content nanoprecipitate dissolution, *Acta Mater.* **296**, 121280 (2025).
- [133] Z. Li, S. Zhao, S. M. Alotaibi, Y. Liu, B. Wang, and M. A. Meyers, Adiabatic shear localization in the CrMnFeCoNi high-entropy alloy, *Acta Mater.* **151**, 424 (2018).
- [134] <https://www.baskerville.ac.uk/>.
- [135] A. A. Maradudin, E. W. Montroll, and G. H. Weiss, Theory of lattice dynamics in the harmonic approximation, in *Solid State Physics* (Academic Press, New York, 1963), Vol. 3.
- [136] G. Leibfried and N. Breuer, Point defects in metals I—Introduction to the theory, in *Springer Tracts in Modern Physics* (Springer-Verlag, Berlin, 1978), Vol. 81.
- [137] V. A. Alshits and V. L. Indenbom, Dynamic dragging of dislocations, *Sov. Phys. Usp.* **18**, 1 (1975).