

Microscopic Mechanisms of Low Lattice Thermal Conductivity in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ Alloys Revealed by Neuroevolution Machine-Learning Potential

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Understanding thermal transport in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys is critical for the reliable thermal management of high-power electronic devices. However, theoretical predictions of lattice thermal conductivity κ_ℓ based on the traditional Abele's virtual crystal approximation (VCA) significantly deviate from experimental measurements, and these discrepancies have long been attributed to finite-size effects. Unlike the traditional VCA, which homogenizes atomic masses and bonding environments, we explicitly incorporate both mass disorder and interatomic force constant (IFC) disorder by directly performing Boltzmann transport equation calculations on large special quasirandom structures, aiming to uncover their impact on lattice thermal transport. Our results show that mass disorder plays a dominant role in suppressing κ_ℓ by significantly enhancing the anharmonic scattering of low-frequency phonons, whereas the heat-carrying capacity of high-frequency phonons is completely eliminated due to substantially reduced group velocities and strong harmonic scattering. In comparison, IFC disorder mainly increases anharmonic scattering rates but has negligible influence on the group velocities of low-frequency phonons. When both disorder types are accounted for, the predicted thermal conductivities align closely with experimental observations. This indicates that the previously reported overestimations from VCA are not due to finite-size effects. We also find that the alloy scattering model based on perturbation theory significantly overestimates the harmonic scattering rates of high-frequency phonons, despite their negligible contribution to thermal conductivity. These findings highlight the necessity of atomistic disorder modeling in wide-bandgap alloys and provide critical insights for thermal design in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ -based electronics.

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I. INTRODUCTION

Aluminum gallium nitride ($\text{Al}_x\text{Ga}_{1-x}\text{N}$) alloys are widely used as essential active materials in high-performance devices, including deep-ultraviolet photodetectors [1,2], high-electron-mobility transistors (HEMTs) [3,4], and ultraviolet lasers [5,6] due to their tunable bandgaps (3.4–6.2 eV) and high breakdown fields (less than 16 MV cm^{-1}) [7,8]. The rapid development of fifth-generation communications and artificial intelligence has driven such devices toward higher operating frequencies

and greater miniaturization, resulting in sharply elevated power densities (approximately 10^4 W cm^{-2}) [9,10]. This imposes severe thermal management challenges and threatens device reliability, particularly in heterostructures such as HEMT barrier layers and superlattice interfaces [11]. Thus, atomistic insights into the phonon transport mechanisms in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys are essential for the rational design of cross-scale thermal management strategies.

Experimentally, the lattice thermal conductivity κ_ℓ of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ has been shown to be drastically suppressed by alloy-induced atomic-scale disorder, including mass fluctuations and variations in bond stiffness. For instance, Liu and Balandin [12,13] reported that the room-temperature κ_ℓ of $\text{Al}_{0.4}\text{Ga}_{0.6}\text{N}$ is reduced by more than 80% relative to that of GaN thin films (approximately $125 \text{ W m}^{-1} \text{ K}^{-1}$). In addition, Tran *et al.* [8,14] observed a pronounced asymmetry in the composition dependence of κ_ℓ , with values decreasing from 115–225 $\text{W m}^{-1} \text{ K}^{-1}$ in GaN to

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$8.8 \text{ W m}^{-1} \text{ K}^{-1}$ in $\text{Al}_{0.57}\text{Ga}_{0.43}\text{N}$. The traditional experimental techniques such as the 3ω method [15] and transient thermoreflectance [8,14] provide macroscopic measurements of thermal conductivity but offer limited insight into microscopic phonon scattering processes.

Theoretically, the thermal conductivity of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ has been computed in several studies [8,14,16] using either the first principles-based Boltzmann transport equation (BTE) or the Callaway model, both in conjunction with Abele's virtual crystal approximation (VCA) [17]. However, these studies [8,14,16] significantly overestimate the thermal conductivity compared with experimental data, often attributing the discrepancy to finite-size or boundary scattering effects. Similar deviations have also been reported in disordered $\text{Si}_x\text{Ge}_{1-x}$ alloys [18], where VCA-based predictions underestimate thermal resistivity at high temperatures. Interestingly, incorporation of explicit mass disorder yields theoretical results that align more closely with experimental measurements across a broad temperature range [18]. This suggests that the long-standing mismatch between theory and experiment in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ may not be solely due to size effects, but may be rather from the fundamental oversight of ignoring realistic atomic-scale disorder, including mass fluctuations and interatomic force constants (IFC) variations.

Accurately capturing atomic-scale disorder, however, poses substantial challenges. First-principles methods offer quantum-level accuracy but become computationally prohibitive for large disordered systems [8,19]. Conversely, empirical potentials are computationally efficient but lack the accuracy needed to model complex many-body interactions because of their simplified and predefined functional forms [20,21]. These limitations have catalyzed the development of machine-learning potentials (MLPs), such as moment tensor potentials (MTPs), deep potentials (DPs), atomic cluster expansion (ACE) [22], and neuroevolution potentials [23–25] (NEPs). Benchmarks have shown that NEPs achieve accuracy in calculating energies, forces, and stresses relative to other state-of-the-art MLPs (e.g., ACE [22], MTPs [26–28], and DPs [29]), simultaneously offering substantially higher computational efficiency owing to their neural-network architecture containing only a single hidden layer together with native graphics-processing-unit implementation. This balance makes NEPs particularly well suited for large-scale simulations of thermal transport in alloys, where both accuracy and efficiency are essential. NEPs have already demonstrated excellent predictive power in disordered $\text{Sc}_x\text{Al}_{1-x}\text{N}$ alloys [30], AlN /diamond interfaces [31], and large-scale radiation damage simulations [32], highlighting their capability to model complex material systems and motivating us to use them for $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys.

In this study, we systematically explore how atomic-scale disorder—specifically, mass and IFC disorder—impact κ_ℓ of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys. Our results demonstrate

that conventional VCA significantly underestimates phonon scattering rates, particularly in the low-frequency range (below 5 THz), leading to overestimation of thermal conductivity by 52%–131%. In contrast, explicit incorporation of both disorder types yields results that closely match experimental data. Although our framework ignores elastic scattering contributions from IFC disorder, equilibrium molecular dynamics (EMD) simulations confirm that this omission has a negligible effect in the dominant phonon frequency range (below 3 THz). However, at higher frequencies (greater than 10 THz), alloy scattering (AS) models based on perturbation theory fail to capture phonon behavior accurately. These findings highlight the importance of modeling realistic disorder and demonstrate the power of high-fidelity MLPs in bridging atomic-scale complexity and macroscopic thermal transport, and in offering critical theoretical insights for optimizing thermal management in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ -based electronics.

II. COMPUTATIONAL METHOD

A. DFT calculations for generating the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ training dataset

In this study, density functional theory (DFT) calculations were with the Vienna Ab initio Simulation Package [33] to construct the training dataset for the NEP developed in this study. The projector-augmented-wave method [34,35] was used to describe the interactions between ionic cores and valence electrons, whereas $2s^22p^3$, $3s^23p^1$, and $4s^23d^{10}4p^1$ were considered as the valence electron configurations of N, Al, and Ga, respectively. The exchange-correlation energy was treated within the generalized gradient approximation [36] using the Perdew-Burke-Ernzerhof functional [35]. The kinetic energy cutoff for the plane-wave basis was set at 600 eV. The Brillouin zone (BZ) was sampled with use of a Γ -centered Monkhorst-Pack [37] grid with a $\mathbf{k}$ -point density of approximately $0.03 \times 2\pi \text{ \AA}^{-1}$, and Gaussian smearing (0.05 eV) was used for the BZ integration. The threshold of the self-consistent-field calculations was set to be 10^{-7} eV.

B. Construction of the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ training dataset for thermal transport studies

For the theoretical investigations of thermal transport properties, a comprehensive training dataset for $\text{Al}_x\text{Ga}_{1-x}\text{N}$ comprising 7194 configurations was meticulously constructed on the basis of an active learning strategy. The dataset covers a variety of atomic configurations, including the crystal structures of AlN and GaN at different temperatures and pressures, homostructural polymorphs obtained from RG^2 [38] searches, and $\text{Al}_x\text{Ga}_{1-x}\text{N}$ crystalline configurations generated via Monte Carlo simulations combined with molecular dynamics (MD) or random substitution methods. In addition, our dataset also

contains liquid amorphous configurations produced by high-temperature melting, structural data retrieved from the Materials Project [39], surface and defect configurations, and solid-solid and solid-liquid interfaces involving AlN/AlN, AlN/GaN, and GaN/GaN systems under various temperatures. This diverse collection provides extensive support for NEP training and also ensures that the model can accurately capture the thermal transport behavior of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ materials under diverse conditions, thereby increasing its predictive accuracy and generalization capability.

C. NEP training

NEP [23–25] is a machine learning–based interatomic potential model that uses neural networks to characterize atomic environments and uses separable natural evolution strategies (SNES) for training. The total energy of the system is expressed as [23–25]

$$U_{\text{total}} = \sum_{i=1}^N U_i, \quad (1)$$

where N is the total number of atoms and U_i is the potential energy of atom i . Each U_i is computed with the use of a feedforward neural network with a single hidden layer, as described in Refs. [23–25]:

$$U_i = \sum_{\mu=1}^{N_{\text{neu}}} w_{\mu}^{(1)} \tanh \left(\sum_{\nu=1}^{N_{\text{des}}} w_{\mu\nu}^{(0)} q_{\nu} - b_{\mu}^{(0)} \right) - b^{(1)}, \quad (2)$$

where $w_{\mu\nu}^{(0)}$ and $w_{\mu}^{(1)}$ denote the weight matrices between the input and hidden layers, and the hidden and output layers, respectively, and $b_{\mu}^{(0)}$ and $b^{(1)}$ represent the bias parameters for the hidden and output layers, respectively. The hidden layer contains N_{neu} neurons, and q_{ν} represents the descriptor vector comprising multiple radial and angular components to describe the local atomic environment. During the training, NEP uses SNESs to minimize the loss function [23–25]:

$$L = \lambda_e L_e + \lambda_f L_f + \lambda_v L_v + \lambda_1 L_1 + \lambda_2 L_2, \quad (3)$$

where L_e , L_f , and L_v are the root mean square errors (RMSEs) for energy, force, and stress predictions, respectively, and λ_e , λ_f , and λ_v are the corresponding weighting factors. L_1 and L_2 are regularization terms with coefficients λ_1 and λ_2 . These are introduced to prevent overfitting and improve the generalization ability of the potential. Further technical details of NEP training are provided in Refs. [24,25]. The specific hyperparameters used in this study are summarized in Table I.

TABLE I. Hyperparameters used for NEP training.

Keyword	Parameter value
type	3 Al Ga N
version	4
cutoff	5 5
use_typewise_cutoff	2.4 2.0
n_max	8 8
basis_size	12 12
l_max	4 2 0
neuron	60
batch	8000
population	50
zbl	2.0
use_typewise_cutoff_zbl	0.65
generation	500 000

D. Calculation of lattice thermal conductivity via the BTE

The lattice thermal conductivities of AlN, GaN, and $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys were computed with the BTE as implemented in ShengBTE [40,41]. In this approach, lattice dynamics are accurately described by incorporating second-order (harmonic) and third-order (anharmonic) IFCs. All IFCs were calculated by the finite-displacement method, and the van der Waals interactions were corrected with the DFT-D3 [42,43] (Becke-Johnson) scheme. Second-order and third-order IFCs were obtained with use of the PHONOPY package [44] and the `thirdorder_vasp.py` [40] script, respectively. For AlN and GaN crystals, $4 \times 4 \times 3$ supercells were used to compute the second-order and third-order IFCs, with a cutoff radius of 6 Å for the third-order interactions.

For $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys, a common theoretical approach is the VCA [8,14,16,45], in which the disordered alloy is replaced by an ordered crystal whose atomic masses, lattice constants, and force constants are interpolated according to the alloy composition. This “virtual” crystal allows the phonon modes to be calculated with the use of a minimal unit cell (u.c.), significantly reducing the computational cost. In many studies, the effects of disorder—such as mass fluctuations—are incorporated in a perturbative manner by adding additional phonon scattering terms (e.g., alloy scattering, as described later) to the calculated phonon lifetimes of the virtual crystal. However, it is worth noting that this approach does not account for the impact of the random distribution of atomic masses and bonding environments present in real disordered alloys. To incorporate the impact of the random distribution of atomic masses and bonding environments, we computed the thermal conductivity using large 96-atom special quasirandom structures (SQSs) [46,47], which incorporate atomic-scale disorder explicitly.

Building upon this, we constructed four distinct schemes that explicitly include alloy scattering, treated analogously to isotope scattering. These schemes—mOfO (with AS), mOfD (with AS), mDfO (with AS), and mDfD (with AS)—represent different combinations of atomic mass (“m”) and force constant (“f”) treatment, with “O” denoting ordered and “D” denoting disordered. Specifically, mOfO (with AS) uses fully averaged lattice constants, atomic masses, and IFCs, consistent with the conventional VCA strategy, and therefore allows the thermal conductivity to be calculated on a four-atom unit cell. In contrast, mOfD (with AS) uses averaged masses but explicit IFCs extracted from 96-atom SQS configurations to account for local bonding stiffness fluctuations; mDfO (with AS) introduces mass disorder (via SQSs) while retaining averaged IFCs, and mDfD explicitly incorporates both mass disorder and IFC disorder. Thus, mOfD (with AS), mDfO (with AS), and mDfD (with AS) adopt full 96-atom SQS configurations to faithfully represent atomic-scale disorder in the alloy. Among these schemes, mDfO (with AS) and mDfD (with AS) share the same mass disorder configuration, while mOfD (with /AS) and mDfD (with AS) used the same set of IFCs. Moreover, although mOfO (with AS) and mDfO (with AS) differ in supercell size, they share the same averaged IFCs in principle. Through comparisons among these four schemes, we can separately identify the effects of mass disorder and IFC disorder, as well as evaluate their combined effect. Notably, for the 96-atom SQS alloy configurations, $2 \times 2 \times 2$ and $1 \times 1 \times 1$ supercells were used to compute the second-order and third-order IFCs, respectively, and the third-order interaction cut-off radius was reduced to 5 Å to balance computational cost and accuracy. The results of the corresponding convergence tests are provided in Fig. S1 in Supplemental Material [48].

The lattice thermal conductivity tensor $\kappa_{\alpha\beta}$ was calculated with the following expression [40]:

$$\kappa_{\alpha\beta} = \frac{1}{k_B T^2 N V} \sum_{\lambda} (\hbar \omega_{\lambda})^2 f_{\lambda}^0 (1 + f_{\lambda}^0) v_{\lambda}^{\alpha} F_{\lambda}^{\beta}, \quad (4)$$

where k_B denotes the Boltzmann constant, T is the absolute temperature, N is the number of $\mathbf{q}$ points sampled in the first Brillouin zone, and V is the unit cell volume. The phonon mode λ is characterized by the wave vector $\mathbf{q}$ and branch index p . The equilibrium Bose-Einstein distribution function is denoted as f_{λ}^0 . v_{λ}^{α} denotes the group velocity of phonon mode λ along the α direction, and F_{λ}^{β} denotes the phonon mean free displacement obtained by solving the linearized BTE.

For pure AlN and GaN crystals, the BTE was solved by a fully iterative method to self-consistently determine the phonon mean free displacement, enabling accurate calculation of normal phonon contributions to lattice thermal

conductivity, and described as [40]

$$\mathbf{F}_{\lambda} = \tau_{\lambda}^0 (\mathbf{v}_{\lambda} + \mathbf{\Delta}_{\lambda}), \quad (5)$$

where τ_{λ}^0 is the relaxation time under the relaxation time approximation (RTA) and $\mathbf{\Delta}_{\lambda}$ is the correction term accounting for deviations from the RTA.

In $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys, strong mass-disorder scattering significantly shortens phonon lifetimes, making resistive scattering processes dominant. Under these conditions, the difference between RTA and full iterative solutions becomes negligible [less than 0.5%; see Fig. S2(a) in Supplemental Material [48]]. Nonetheless, even within the RTA framework, the number of three-phonon scattering processes in a 96-atom supercell can easily reach hundreds of millions, rendering the calculation extremely demanding. Recently, a maximum likelihood sampling approach was developed [41] to accelerate the evaluation of phonon scattering rates. Instead of evaluating all scattering processes, this method computes only a small random subset (typically 0.013%–6.25% of the total) and statistically reconstructs the overall scattering rates. This strategy reduces the computational cost by several orders of magnitude while keeping the error within a few percent. For example, in the case of 96-atom $\text{Al}_{0.125}\text{Ga}_{0.875}\text{N}$ alloy, only 10^6 scattering processes were computed out of approximately 8.373×10^9 total processes, achieving an error in the predicted value of the lattice thermal conductivity below 1% [see Fig. S2(b) in Supplemental Material [48]]. Therefore, we used this method to efficiently evaluate the phonon scattering rates in large alloy supercells.

The alloy elastic scattering rate of phonon mode λ was calculated by analogy with isotope scattering as [16,49,50]

$$\tau_{\lambda, \text{AS}}^{-1} = \frac{1}{N} \sum_{\lambda'} \Gamma_{\lambda\lambda'}, \quad (6)$$

where N is the number of sampled $\mathbf{q}$ points and $\Gamma_{\lambda\lambda'}$ is the elastic scattering probability from phonon mode λ to phonon mode λ' , given by [16,49,50]

$$\Gamma_{\lambda\lambda'} = \frac{\pi \omega_{\lambda}^2}{2} \sum_{i \in \text{u.c.}} g(i) |\mathbf{e}_{\lambda}^*(i) \cdot \mathbf{e}_{\lambda'}(i)|^2 \delta(\omega_{\lambda} - \omega_{\lambda'}). \quad (7)$$

$g(i)$ is the mass-variance parameter, defined as

$$g(i) = \sum_s f_s(i) [1 - M_s(i)/\bar{M}(i)]^2, \quad (8)$$

where $f_s(i)$ and $M_s(i)$ are the concentration and mass of the s th alloying element at the i th atomic site, respectively, and $\bar{M}(i)$ is the average mass at site i . $\mathbf{e}_{\lambda}(i)$ denotes the phonon eigenvector component. The δ function $\delta(\omega_{\lambda} - \omega_{\lambda'})$ ensures energy conservation of the two-phonon process.

The intrinsic anharmonic scattering rate of phonon mode λ was evaluated from three-phonon absorption and emission processes as [40,41]

$$\tau_{\lambda,\text{anh}}^{-1} = \frac{1}{N} \left(\sum_{\lambda'\lambda''}^+ \Gamma_{\lambda\lambda'\lambda''}^+ + \frac{1}{2} \sum_{\lambda'\lambda''}^- \Gamma_{\lambda\lambda'\lambda''}^- \right), \quad (9)$$

where the superscripts “+” and “−” denote absorption and emission processes, respectively. The corresponding three-phonon scattering probabilities are given by

$$\Gamma_{\lambda\lambda'\lambda''}^+ = \frac{\hbar\pi}{4} \frac{f_{\lambda'}^0 - f_{\lambda''}^0}{\omega_{\lambda}\omega_{\lambda'}\omega_{\lambda''}} |V_{\lambda\lambda'\lambda''}^+|^2 \delta(\omega_{\lambda} + \omega_{\lambda'} - \omega_{\lambda''}) \quad (10)$$

and

$$\Gamma_{\lambda\lambda'\lambda''}^- = \frac{\hbar\pi}{4} \frac{f_{\lambda'}^0 + f_{\lambda''}^0 + 1}{\omega_{\lambda}\omega_{\lambda'}\omega_{\lambda''}} |V_{\lambda\lambda'\lambda''}^-|^2 \delta(\omega_{\lambda} - \omega_{\lambda'} - \omega_{\lambda''}), \quad (11)$$

where f_{λ}^0 is the equilibrium Bose-Einstein occupation number of phonon mode λ and $V_{\lambda\lambda'\lambda''}^{\pm}$ is the three-phonon scattering matrix element calculated from the third-order IFCs,

$$V_{\lambda\lambda'\lambda''}^{\pm} = \sum_{i \in \text{u.c.}} \sum_{j,k} \sum_{\alpha\beta\gamma} \Phi_{ijk}^{\alpha\beta\gamma} \frac{e_{\lambda}^{\alpha}(i) e_{\lambda'}^{\beta}(\pm \mathbf{q}') e_{\lambda''}^{\gamma}(\mp \mathbf{q}'')}{\sqrt{M_i M_j M_k}}, \quad (12)$$

where $\Phi_{ijk}^{\alpha\beta\gamma}$ is the third-order IFC tensor, M_i is the atomic mass, and $e_{\lambda}^{\alpha}(i)$ is the phonon eigenvector component of atom i along the Cartesian direction α . The δ functions enforce energy conservation, while momentum conservation is imposed in the summations over the allowed three-phonon processes. Within the BTE framework, the total scattering rate of phonon mode λ in the alloy system is then written as

$$\tau_{\lambda,\text{total}}^{-1} = \tau_{\lambda,\text{AS}}^{-1} + \tau_{\lambda,\text{anh}}^{-1}. \quad (13)$$

In the calculations labeled as “with AS,” both $\tau_{\lambda,\text{AS}}^{-1}$ and $\tau_{\lambda,\text{anh}}^{-1}$ were included. In contrast, in the calculations labeled as “without AS,” only $\tau_{\lambda,\text{anh}}^{-1}$ was retained.

It is worth noting that, beyond the elastic scattering term (i.e., $\Gamma_{\lambda\lambda'}$) arising from mass disorder, contributions from IFC disorder should also be considered in principle [51]. However, this term was not explicitly included in our calculations, as its impact can be considered negligible for $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys. As demonstrated later through Eqs. (18)–(22), the perturbation associated with IFC disorder is much weaker than that associated with mass disorder. Moreover, this conclusion is further supported by the consistency between the BTE and molecular dynamics results.

E. Calculation of lattice thermal conductivity via the HNEMD method

The homogeneous nonequilibrium molecular dynamics (HNEMD) [52,53] method was used to compute κ_{ℓ} , as implemented in the GPUMD package [23]. In this method, each atom i experiences an additional nonconservative force, defined as [52]

$$\mathbf{F}_i^{\text{ext}} = E_i \mathbf{F}_e + \mathbf{W}_i \cdot \mathbf{F}_e, \quad (14)$$

where E_i is the total energy of atom i , $\mathbf{F}_e$ is the external driving force parameter, and $\mathbf{W}_i$ is the virial tensor, defined as

$$\mathbf{W}_i = \sum_{j \neq i} \left(\frac{\partial U_j}{\partial \mathbf{r}_{ji}} \otimes \mathbf{r}_{ij} \right), \quad (15)$$

where U_i is the potential energy of atom i and $\mathbf{r}_{ij}$ is the displacement vector from atom i to atom j . In the HNEMD framework, the ensemble-averaged heat flux $\langle J_{\alpha}(t) \rangle_{ne}$ is related to the driving force F_e^{β} through

$$\frac{\langle J_{\alpha}(t) \rangle_{ne}}{TV} = \sum_{\beta} \kappa^{\alpha\beta} F_e^{\beta}. \quad (16)$$

The driving force magnitude must be selected carefully to remain within the linear response regime while ensuring a sufficiently high signal-to-noise ratio [52,54]. In this study, the driving force parameter was set to be 0.1 and 0.2 μm^{-1} for the SQS-expanded and directly randomized supercells of the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloy, respectively. The time step was set to 1 fs. For each system, molecular dynamics simulations were first equilibrated in the NPT ensemble at 300 K and 0 GPa with the use of a Nosé-Hoover thermostat for 500 000 steps, followed by a further equilibration in the NVT ensemble for another 500 000 steps. After equilibration, the HNEMD simulations were performed for 5 000 000 steps to calculate κ_{ℓ} .

III. RESULTS AND DISCUSSION

A. Development and training accuracy of the NEP for $\text{Al}_x\text{Ga}_{1-x}\text{N}$ systems

Figure 1 illustrates the active learning framework used for training the NEP in the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ system, along with uniform manifold approximation and projection (UMAP)-based visualization of the configuration space of the training sets. As shown in Fig. 1(a), the training follows an iterative optimization scheme. The initial dataset is generated by molecular dynamics simulations with empirical potentials, manual configuration perturbations, and physics-informed selection strategies. DFT calculations are then performed to obtain the total energies, forces, and stress tensors to build the reference dataset for the

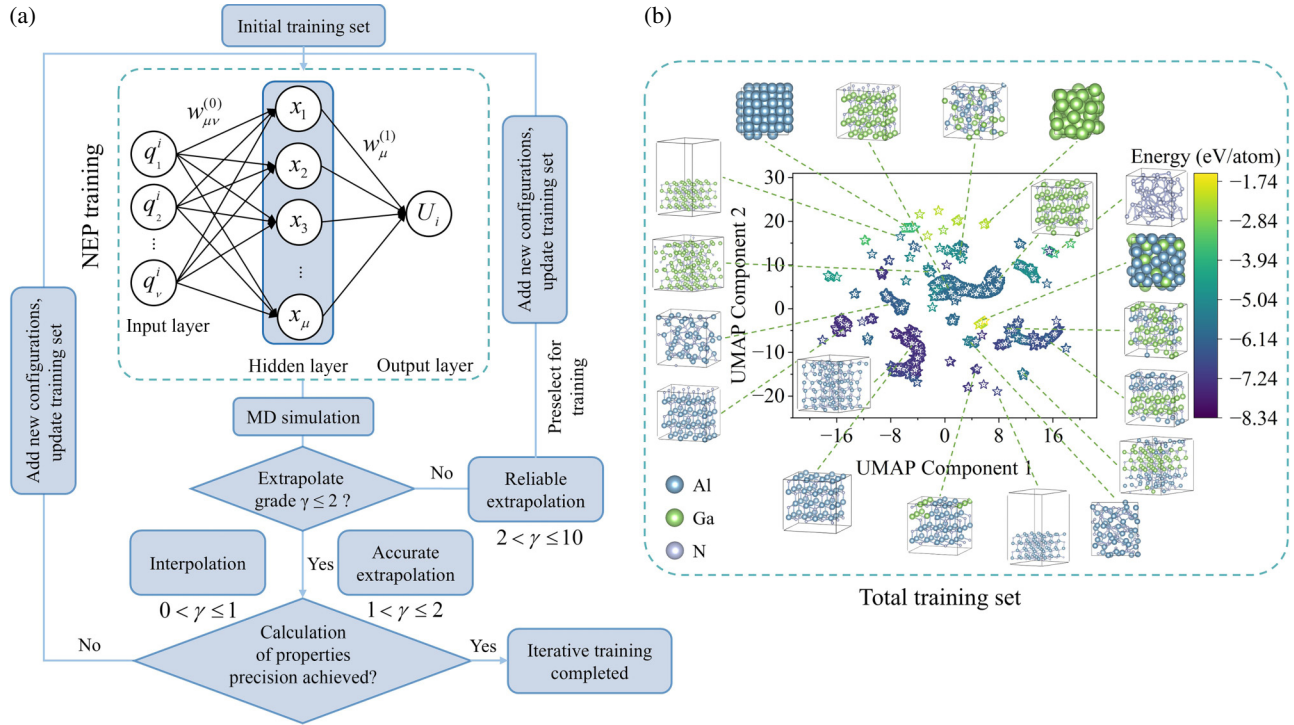


FIG. 1. Active training framework and configuration space visualization of the training set for the neuroevolution machine-learning potential developed for the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ system. (a) NEP active training process. (b) UMAP-based dimensionality-reduction visualization of configuration space distribution and energy characteristics. Representative structures (including crystalline, amorphous, and surface configurations) are highlighted with dashed lines indicating their positions in the feature space.

initial training of the model. The model is subsequently refined through the active learning loop based on the D-optimality criterion [70,71] and the MaxVol algorithm [72]. The extrapolation indicator γ , which quantifies the degree of model extrapolation for a given configuration or its neighborhood, is defined as [71,73]

$$\gamma(cfg) = \max_{1 \leq j \leq m} |c_j|, \quad \text{where } (c_1 \cdots c_m) = \mathbf{b}A^{-1}, \quad (17)$$

where $\mathbf{b}$ is the parameter-gradient vector of the candidate configuration and A is the parameter-gradient matrix of the current active set composed of the most informative configurations selected during training. Thus, γ measures how strongly the candidate configuration is extrapolated beyond the domain spanned by the active set. More detailed descriptions of the extrapolation indicator and its implementation can be found in Refs. [71,73]. Configurations with $\gamma \leq 1$ are considered within the safe interpolation region; $1 < \gamma \leq 2$ corresponds to a controllable extrapolation region; $\gamma > 2$ signifies a high-risk extrapolation state. By the setting of a threshold of $\gamma = 2$, the system automatically identifies configurations near the model's predictive boundary (such as interfaces, defects, and dislocation cores) for DFT calculations, which are then incorporated into the training set for targeted enhancement. To ensure both reliability and generalization, the

training process enforced two convergence criteria, i.e., (1) all configurations in the target MD trajectories must have extrapolation indicators γ below the reliability threshold and (2) the predictions of key physical properties, such as lattice constants, phonon spectra, elastic constants, and κ_ℓ , must remain accurate at each iteration. In addition, L_1 and L_2 regularizations were applied during each training iteration to constrain model weight parameters, prevent overfitting, and enhance generalization. This iterative “sampling-training-validation” scheme progressively refines the potential while maintaining balance between the model complexity and physical fidelity across diverse phase spaces. Figure 1(b) visualizes the configuration space of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ generated with the UMAP method, and reveals the distinct clustering of crystalline, amorphous, and surface structures in the reduced manifold.

The NEP training process and its predictive accuracy are depicted in Fig. 2. As shown in Fig. 2(a), the loss function steadily converges with the increasing training steps. Excellent agreement is achieved between the DFT-calculated results and the predicted values of total energies, forces, and stress tensors [shown in Figs. 2(b)–2(d)]. Specifically, the predicted total energy achieves a near-perfect linear correlation with the DFT results, possessing $R^2 = 1.0$ and RMSE of 9.813 meV/atom, while the forces and stresses have RMSEs of 0.239 eV Å⁻¹ and

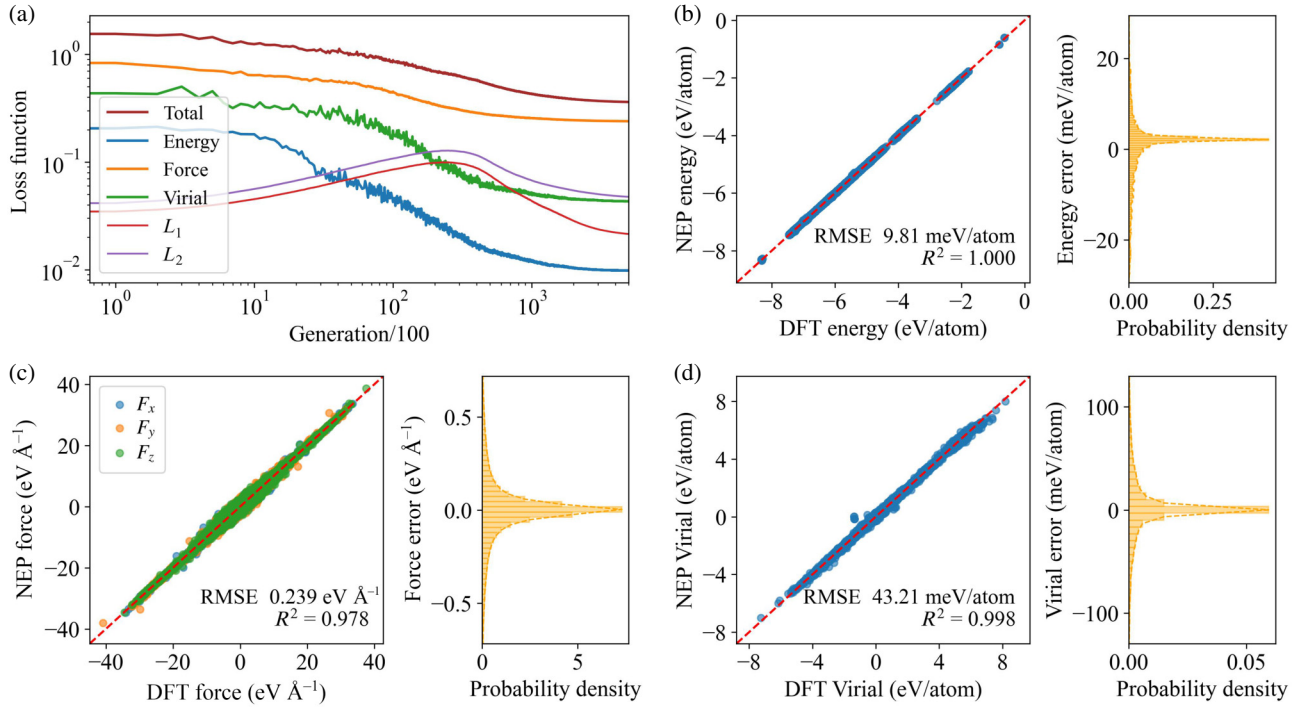


FIG. 2. Training process and prediction accuracy of the NEP. (a) Convergence of the loss function. (b) Accuracy of energy predictions. (c) Accuracy of force predictions. (d) Accuracy of virial predictions. Here the virial is normalized as $W_{\alpha\beta} = \sigma_{\alpha\beta}V/N$, where $\sigma_{\alpha\beta}$ is the stress tensor component, V is the cell volume, and N is the total number of atoms.

43.215 meV/atom, with R^2 values of 0.978 and 0.998, respectively. The relatively large overall force RMSE originates from the deliberately broad training dataset, which includes not only crystalline AlN, GaN, and $\text{Al}_x\text{Ga}_{1-x}\text{N}$ but also amorphous, defective, and interfacial configurations to ensure transferability. For the crystalline phases that are directly relevant to phonon transport, the RMSEs are significantly lower—0.045 eV $\text{\AA}^{-1}$ for AlN, 0.047 eV $\text{\AA}^{-1}$ for GaN, and 0.051 eV $\text{\AA}^{-1}$ for $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys (see Fig. S3 in Supplemental Material [48]), ensuring the fidelity of the NEP for predicting phonon-related properties. In addition, to further confirm model generalization, we performed out-of-sample validations on unseen $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloy compositions. The predicted energies, forces, and virials obtained through the NEP remain in close agreement with DFT references (see Fig. S4 in Supplemental Material [48]), confirming reliable transferability across compositional gradients and diverse local atomic environments. These results demonstrate that the NEP developed can faithfully capture multiple physical quantities, thus establishing a reliable basis for its application to complex material systems.

B. Multiproperty validation of the NEP developed in this work

Accurate prediction of the ground-state configurations is necessary for assessing the interatomic potential. This requires that the potential not only captures

near-equilibrium energy characteristics but also identifies energy extrema during global searches of the potential energy surface. In this study, use of the well-trained NEP was combined with use of the crystal structure search program RG² [38] to comprehensively explore the configuration space of AlN and GaN. As shown in Fig. 3(a), the NEP successfully predicted the ground-state configurations of AlN and GaN as the wurtzite phase. Wurtzite AlN and GaN are strongly polar crystals. Thus, significant local charge redistribution and energy fluctuations during polarization switching impose stringent requirements on the dynamic response accuracy of the potential. Traditional empirical potentials, such as the Stillinger-Weber (SW) potential [74], are constrained by their predefined functional forms and often fail to accurately capture the dynamic evolution of local atomic environments during ferroelectric phase transitions, leading to systematic overestimations of ferroelectric switching energy barriers. In contrast, the NEP accurately reproduces the potential energy surface along the polarization reversal path. The intermediate images were constructed with use of the nudged elastic band method via interpolation between the polarized and oppositely polarized states. As shown in Fig. 3(b), the switching energy barriers computed with the NEP for wurtzite AlN, GaN, and $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$ crystals are in excellent agreement with DFT results.

To further validate the reliability of the NEP in predicting lattice dynamics and mechanical properties, we calculated the phonon dispersion and elastic constants of

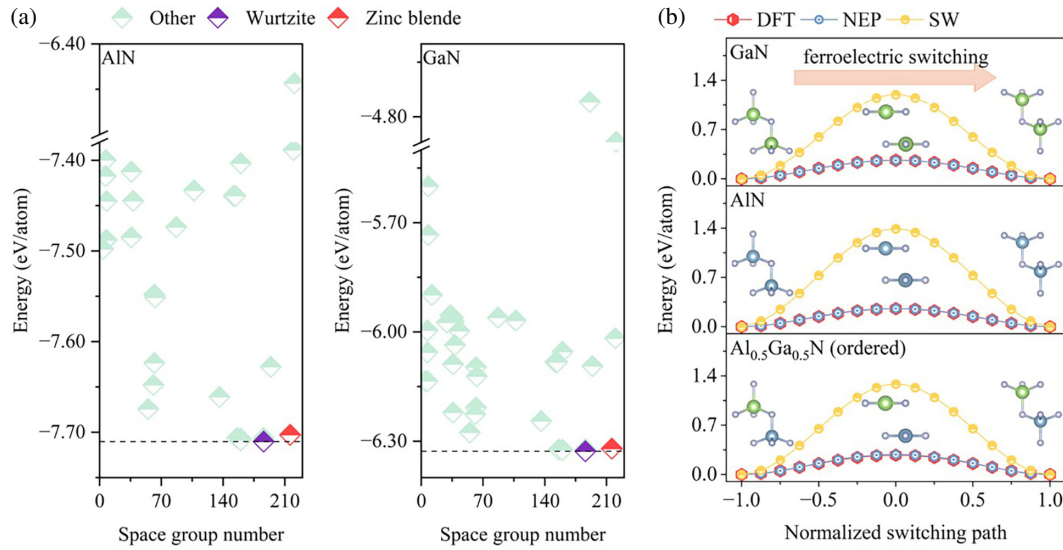


FIG. 3. (a) Ground-state structure prediction for AlN and GaN using the NEP combined with use of the crystal structure search program RG² [38]. (b) Ferroelectric switching energy barriers for AlN, GaN, and Al_{0.5}Ga_{0.5}N crystals calculated with DFT, the NEP, and the SW potential.

AlN, GaN, and Al_{0.5}Ga_{0.5}N crystals. Figures 4(a)–4(c) show that, except for a few high-frequency optical branches along the Γ - A direction, the NEP reproduces the phonon dispersions along the high-symmetry path Γ - K - M - Γ - A reasonably well in comparison with the DFT results. In particular, the maximum optical mode frequencies at the Γ point predicted by the NEP deviate by less than 3% from inelastic x-ray scattering values [55,56] and Raman spectroscopy values [57], whereas the SW potential exhibits systematic overestimation of up to 42% in the high-frequency region. Similarly, the relative errors in the elastic constants C_{11} , C_{12} , C_{33} , C_{44} , and C_{66} of the wurtzite structures predicted by the NEP are below 3%, as shown in Figs. 4(d)–4(f). In contrast, the SW potential exhibits a significant 117% overestimation in C_{33} of AlN, highlighting severe deficiencies in describing the energy associated with tetrahedral bond angle distortions.

In Fig. 5, we compare the temperature-dependent κ_ℓ calculated with the NEP and other methods for AlN and GaN crystals. Experimental results are also provided for reference. Overall, the κ_ℓ values predicted by the NEP show good agreement with previously reported theoretical values [16,20,64–67] and available experimental measurements [58–63], whereas the SW potential significantly overestimates κ_ℓ across the entire temperature range. For example, at 300 K, the NEP-based calculations give $\kappa_a = 344.1 \text{ W m}^{-1} \text{ K}^{-1}$ and $\kappa_c = 289.9 \text{ W m}^{-1} \text{ K}^{-1}$ for AlN, compared with the previously reported DFT-based ranges [64,65] of 301.1–322.3 $\text{W m}^{-1} \text{ K}^{-1}$ and 286.2–295.8 $\text{W m}^{-1} \text{ K}^{-1}$, respectively. For GaN, the calculations give $\kappa_a = 247.1 \text{ W m}^{-1} \text{ K}^{-1}$ and $\kappa_c = 254.7 \text{ W m}^{-1} \text{ K}^{-1}$, compared with the previously reported DFT-based ranges [16,60] of 242–243.9 $\text{W m}^{-1} \text{ K}^{-1}$ and

239–278.6 $\text{W m}^{-1} \text{ K}^{-1}$, respectively. By contrast, the SW-predicted values exceed the experimental observations by approximately 400% and 160% for AlN and GaN, respectively. This anomalous overestimation is attributable to the deviation in the calculated phonon spectrum. As shown in Figs. 4(a)–4(b), the hardening of the phonon branch in the calculated dispersion with the SW potential results in significantly overestimated phonon group velocities and an increased gap in the phonon dispersion, hence reducing scattering channels and extending phonon lifetimes. These combined effects ($\kappa_\ell \propto v_g^2 \tau$) ultimately lead to anomalously high predictions of κ_ℓ . In contrast, the NEP accurately reproduces phonon eigenstates, elastic constants, and thermal transport properties by precisely reconstructing the many-body potential energy surface. This rigorous multiproperty validation of the NEP provides high-confidence computational support for subsequent investigations into the thermal transport mechanisms of Al_xGa_{1-x}N alloys.

C. Thermal transport in disordered Al_xGa_{1-x}N alloys

On the basis of the reliability of the NEP established in the preceding section, we systematically investigated the thermal transport along the c axis of the Al_xGa_{1-x}N alloy considering different compositions, which are critical for heat dissipation in Al_xGa_{1-x}N-based HEMTs [75]. To realistically represent the inherent atomic-scale disorder in the alloy, the SQS method was used to generate three independent configurations of 96 atoms for each aluminum composition ($x = 0.125$ – 0.875), as shown in Fig. S5 in Supplemental Material [48]. The 96-atom cell

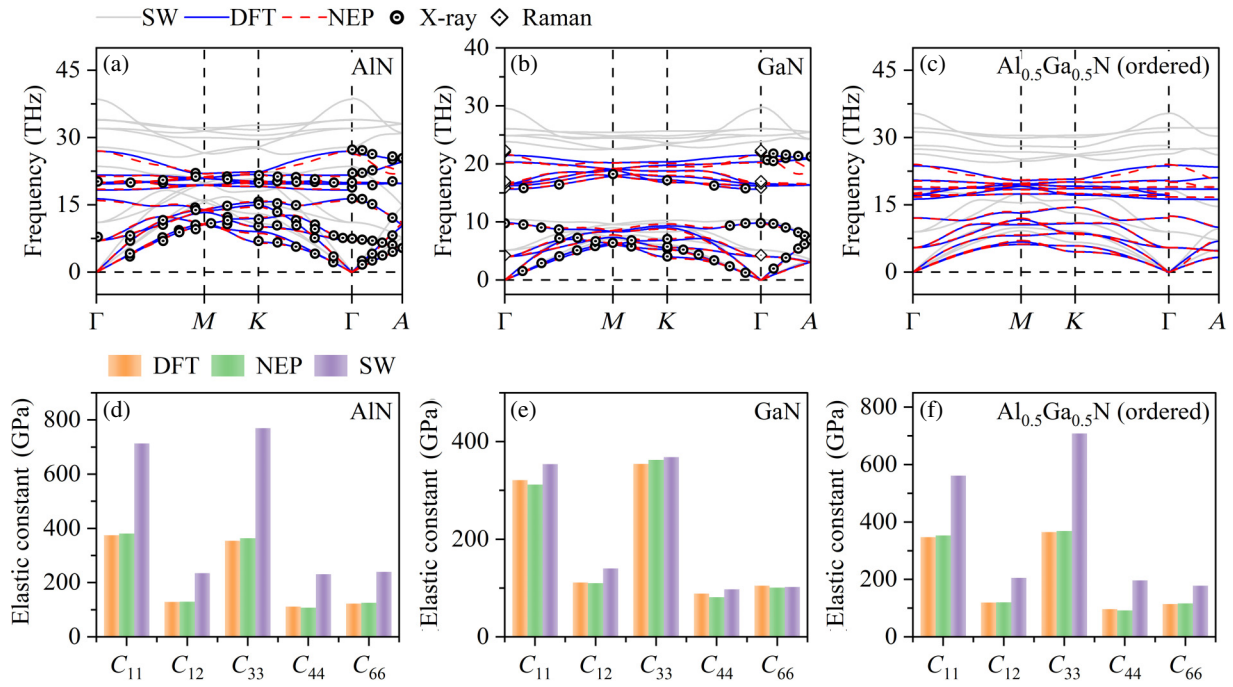


FIG. 4. (a)–(c) Phonon spectra and (d)–(f) elastic constants of AlN, GaN, and $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$ crystals calculated with DFT, the NEP, and the SW potential. Circles and diamonds in (a)–(c) denote experimental data from x-ray scattering [55,56] and Raman spectroscopy [57], respectively.

size was chosen to balance the need for statistical randomness with the computational feasibility of subsequent phonon transport calculations. For each composition, the κ_ℓ values were calculated with the use of three independently generated 96-atom SQS configurations to evaluate the impact of structural randomness on heat transport. The results showed that the variations in κ_ℓ among the three 96-atom SQS configurations were consistently below 1% (see Fig. S6 in Supplemental Material [48]). Consequently, the first 96-atom SQS configuration for each composition was adopted as the reference structure for all subsequent BTE calculations.

Notably, although the 96-atom SQS configurations explicitly incorporate local mass disorder and local IFC disorder into the phonon eigenstates, group velocities, and anharmonic scattering matrix elements, the BTE calculation still underestimates the overall phonon scattering if the alloy elastic scattering term in Eq. (6) is not included. As shown in Fig. 6(a), the calculated κ_ℓ values for these 96-atom SQS configurations without incorporation of alloy elastic scattering [i.e., mDfD (without AS)] are overestimated by a factor of 4–8 in comparison with the experimental values [8,14,68,69]. This effect is directly reflected in the HNEMD results for the periodically replicated 96-atom SQS structure. For example, when the original 96-atom SQS configuration is replicated in a 28 800-atom supercell, κ_ℓ is calculated to be $61.5 \text{ W m}^{-1} \text{ K}^{-1}$, in good agreement with the $62.9 \text{ W m}^{-1} \text{ K}^{-1}$ obtained from

the BTE calculation without inclusion of alloy scattering [mDfD (without AS)]. In contrast, a fully disordered supercell containing 28 800 atoms, generated by the random substitution of Ga atoms for 50% of Al atoms, exhibited significantly lower thermal conductivities, averaging $9.7 \pm 0.8 \text{ W m}^{-1} \text{ K}^{-1}$ across five independent simulations [Figs. 6(c)–6(d)]. The convergence of the HNEMD results with respect to the simulation cell size was also carefully verified (see Fig. S7 in Supplemental Material [48]). This stark contrast highlights the pronounced impact of atomic disorder on phonon transport, and indicates the necessity of including the alloy elastic scattering term in the BTE framework.

It is worth noting that the alloy elastic scattering contribution is not automatically incorporated by simply increasing the SQS supercell size. As shown in Fig. S9 in Supplemental Material [48], κ_ℓ calculated with the mDfD (without AS) scheme gradually converges with increasing SQS supercell size, but the converged value remains much higher than the experimental values. This can be understood from the scattering mechanisms included in the BTE framework. As shown in Eq. (13), the total scattering rate is given by $\tau_{\lambda,\text{total}}^{-1} = \tau_{\lambda,\text{AS}}^{-1} + \tau_{\lambda,\text{anh}}^{-1}$. In the mDfD (without AS) calculations, only the anharmonic scattering term $\tau_{\lambda,\text{anh}}^{-1}$ is included, whereas the alloy elastic scattering term $\tau_{\lambda,\text{AS}}^{-1}$ induced by stochastic mass fluctuations is absent. The observed convergence mainly reflects the convergence of the anharmonic scattering contribution.

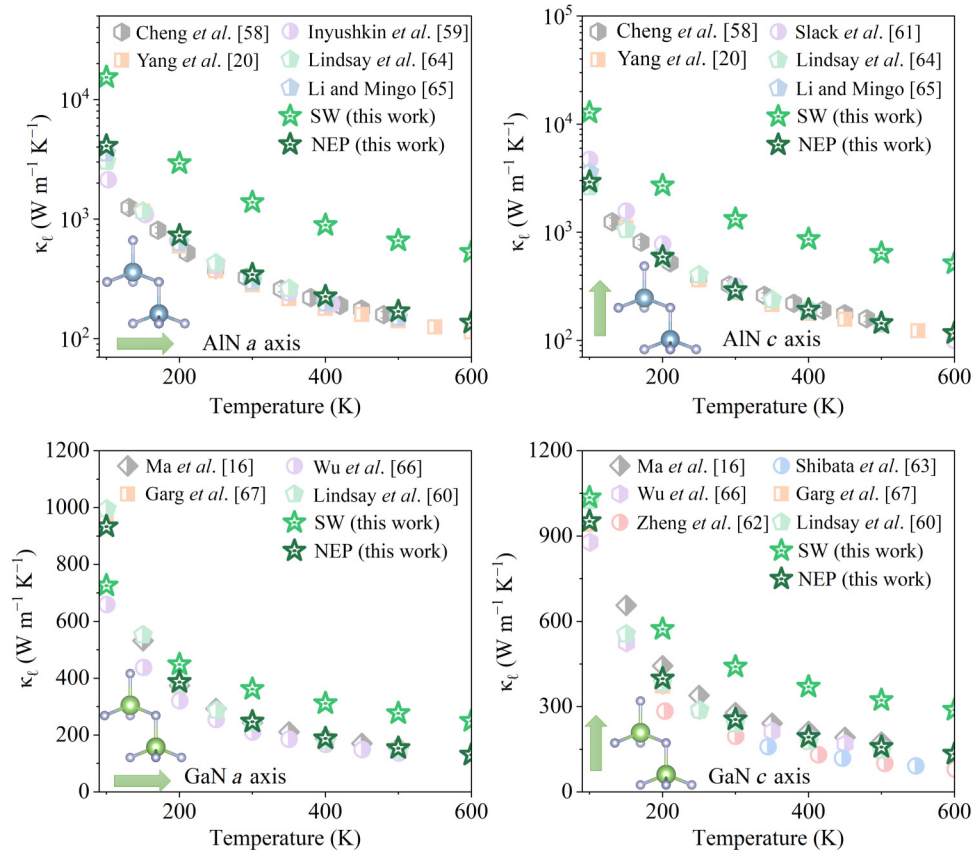


FIG. 5. κ_ℓ of AlN and GaN calculated with the NEP and the SW potential in comparison with previous experimental and theoretical results [16,20,58–67]. The NEP-based and SW-based results in this work were obtained from fully iterative BTE calculations.

Therefore, to more accurately capture the effect of atomic disorder, we used the four schemes introduced in Sec. II: mOfO (with AS), mOfD (with AS), mDfO (with AS), and mDfD (with AS). In all these schemes, the alloy scattering term is included in the BTE framework to correct the overestimation caused by ignoring the alloy elastic scattering term. These schemes differ in how atomic masses and force constants are treated, enabling a comparative analysis of their effects on phonon group velocities, scattering rates, and ultimately thermal conductivity. The convergence of calculated κ_ℓ with respect to both the $\mathbf{q}$ -point sampling and SQS supercell size was carefully verified (see Figs. S8 and S9 in Supplemental Material [48]). As shown in Fig. 7(a), compared with the mDfD (without AS) scheme discussed above, mOfO (with AS) yields a significantly reduced κ_ℓ , yet it still remains considerably higher than the experimental measurements. This overestimation is attributed primarily to the simple averaging of atomic masses and IFCs, which fails to capture the true distribution of mass disorder in real alloys. A similar limitation was also observed in previous studies, where conventional VCA calculations significantly overestimated κ_ℓ of $\text{Si}_x\text{Ge}_{1-x}$ alloys [18] at high temperatures due to the lack of explicit mass disorder. Notably, that

study considered only mass disorder, and ignored IFC disorder. However, our results show that IFC disorder also plays a critical role in suppressing thermal transport in the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloy system.

To further quantify the role of each type of disorder, we compared the individual effects of IFC disorder and mass disorder, as shown in Fig. 7(b). The introduction of either IFC disorder [mOfD (with AS)] or mass disorder [mDfO (with AS)] substantially enhances phonon scattering, resulting in a marked reduction in thermal conductivity. Specifically, the thermal conductivity of $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$ alloy decreases from $21.5 \text{ W m}^{-1} \text{ K}^{-1}$ [mOfO (with AS)] to $13.3 \text{ W m}^{-1} \text{ K}^{-1}$ [mOfD (with AS)] when only IFC disorder is included, and decreases further to $10.8 \text{ W m}^{-1} \text{ K}^{-1}$ [mDfO (with AS)] when only mass disorder is included. Notably, when both mass disorder and IFC disorder are considered simultaneously [mDfD (with AS)], κ_ℓ of the $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$ alloys further reduces to $10.1 \text{ W m}^{-1} \text{ K}^{-1}$, and the predicted values are closer to the experimental results across the full range of alloy composition. The greater reduction observed in the mass-disordered case indicates that for the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloy system, mass disorder plays a more dominant role in phonon scattering.

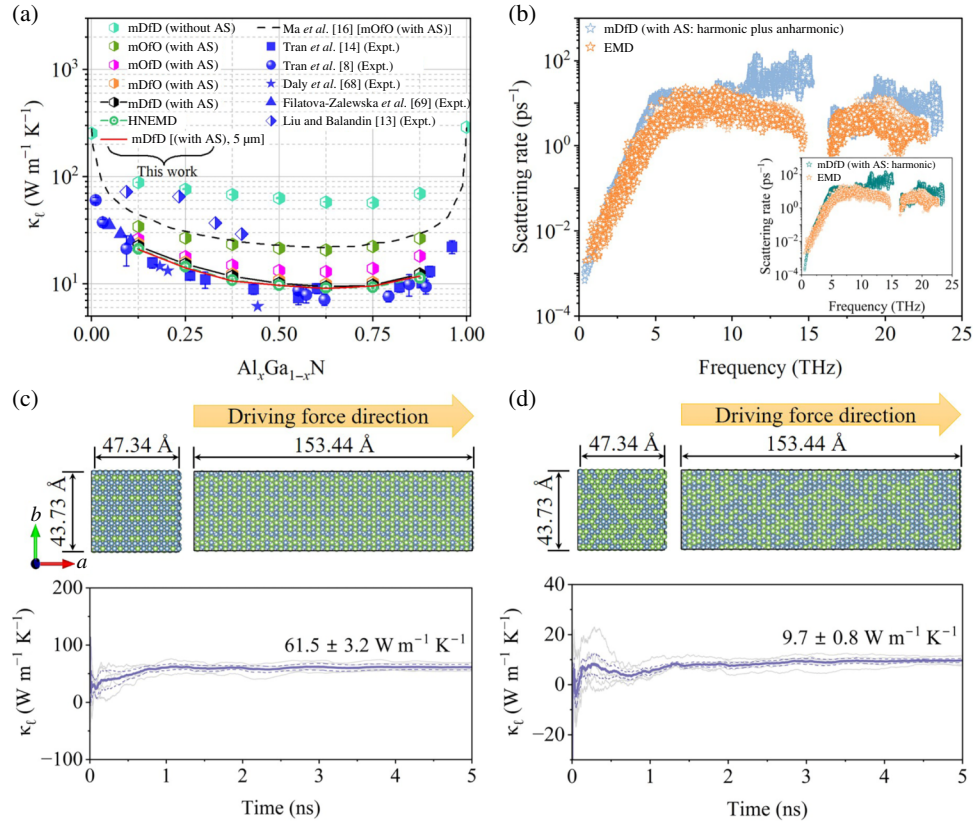


FIG. 6. Thermal transport properties of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ disordered alloys at 300 K. (a) Composition dependence of κ_ℓ calculated by HNEMD and with the following schemes: mDfD (without AS), mOfO (with AS), mOfD (with AS), mDfO (with AS), and mDfD (with AS). For mDfD (with AS), results accounting for finite-size effects with a phonon mean free path cutoff of 5 μm are also shown. Results are compared with experimental data and previous theoretical data [8,13,14,16,68,69]. (b) Phonon scattering rates of $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$ calculated by mDfD (with AS) and EMD methods (with 92 160 atoms in a simulation cell of approximately $10.10 \times 9.84 \times 10.22 \text{ nm}^3$) at 300 K. (c) κ_ℓ of $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$ computed by HNEMD with an SQS-expanded supercell, in which 50% of Al atoms are replaced by Ga atoms in a 96-atom SQS supercell and periodically expanded. (d) Results for a directly randomized supercell of the same size as in (c), where 50% of Al atoms are randomly replaced by Ga atoms. Gray lines show five independent simulations; the purple line and the dashed region denote the average error and the standard error.

The stronger impact of mass disorder can be qualitatively understood from the perspective of phonon-defect scattering within the T -matrix formalism, where the defect-phonon interaction is described by a perturbation matrix V constructed in real space. The corresponding phonon-defect scattering rate is expressed as [76,77]

$$\tau_{\lambda,\text{def}}^{-1} = \pi \chi_{\text{def}} \frac{\Omega}{V_{\text{def}} \omega_\lambda} \frac{1}{\sum_{\lambda'}} |\langle \lambda' | T | \lambda \rangle|^2 \delta(\omega_{\lambda'}^2 - \omega_\lambda^2), \quad (18)$$

where $\lambda = (j, \mathbf{q})$ denotes a phonon mode, χ_{def} is the number fraction of defects, V_{def} is the volume of a defect, Ω is the normalization volume, and ω_λ is the phonon angular frequency. Here, $T = (I - Vg^+)^{-1}V$ is the T -matrix, the matrix bridging the Green's function between perturbed and unperturbed systems. I is the identity matrix, and g^+ is the causal Green's function of the perfect crystal. In the Born approximation, $T \approx V$, which is justified by the expansion $T = V + Vg^+V + \dots$ [78]. The perturbation

matrix V can be decomposed into two contributions associated with mass and IFC variations between the perfect and defective structures [76,77]:

$$\begin{aligned} V_M^{i\alpha,j\beta} &= -\left(\frac{M'_i}{M_i} - 1\right) \omega_\lambda^2 \delta_{ij} \delta_{\alpha\beta}, \\ V_K^{i\alpha,j\beta} &= \frac{K'_{i\alpha,j\beta} - K_{i\alpha,j\beta}}{\sqrt{M_i M_j}}, \end{aligned} \quad (19)$$

where i and j are atomic indices and $\alpha, \beta \in \{x, y, z\}$. M_i and M'_i denote the masses of the original and defect atoms at the i th site, respectively, and K and K' are the second-order IFCs of the perfect and defective structures. Since V_M scales with ω_λ^2 , V_K can be reformulated in the same form for direct comparison. Note that in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys, the diagonal on-site elements ($i = j$, $\alpha = \beta$) are significantly larger than the off-diagonal terms. Thus, K' can be

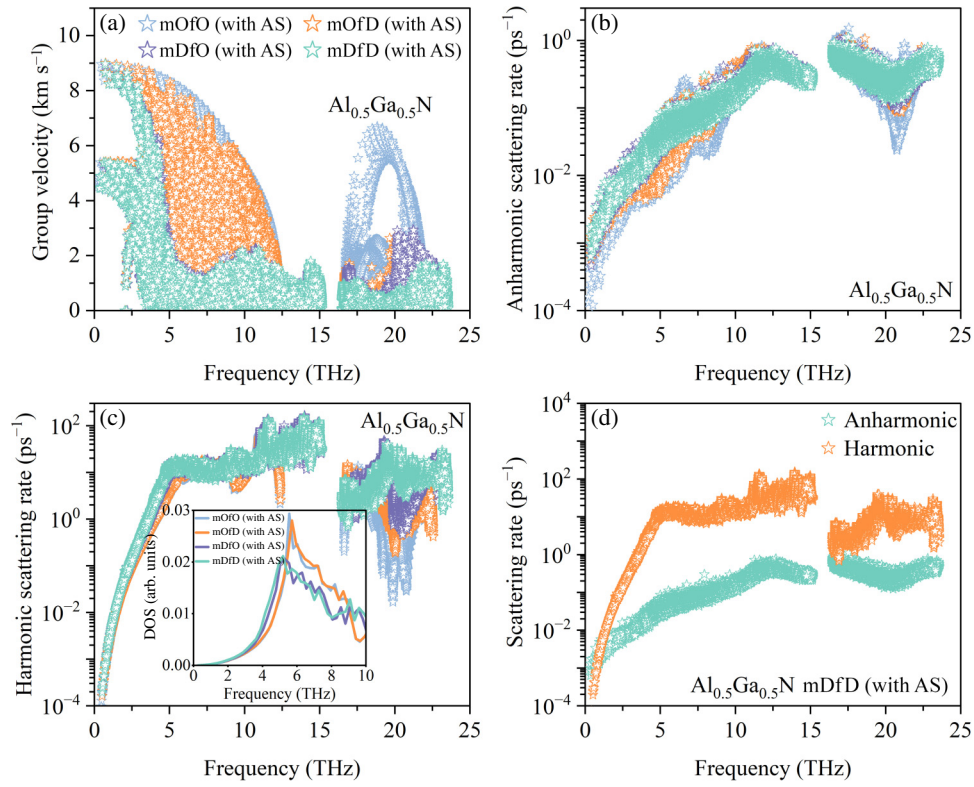


FIG. 7. Phonon thermal transport properties of the $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$ disordered alloy calculated with four disorder schemes [mOfO (with AS), mOfD (with AS), mDfO (with AS), and mDfD (with AS)] at 300 K. (a) Phonon group velocity. (b) Anharmonic scattering rate. (c) Harmonic scattering rate and normalized phonon density of states (DOS). (d) Comparison of harmonic and anharmonic scattering rates in the mDfD (with AS) scheme.

roughly estimated as $K' \approx a_{K'}K$, with

$$a_{K'} = \sum_{i=j, \alpha=\beta} |K'_{i\alpha,j\beta}| / \sum_{i=j, \alpha=\beta} |K_{i\alpha,j\beta}|. \quad (20)$$

Consequently,

$$\begin{aligned} V_K^{i\alpha,j\beta} &\approx \frac{(a_{K'} - 1)K_{i\alpha,j\beta}}{\sqrt{M_i M_j}} \\ &\approx (a_{K'} - 1)\omega_\lambda^2 \delta_{ij} \delta_{\alpha\beta}. \end{aligned} \quad (21)$$

By using Eq. (20), we obtain $K^{\text{GaN}} = 0.85K^{\text{AlN}}$, whereas $M_{\text{Ga}} = 2.58M_{\text{Al}}$. This contrast clearly shows that the perturbation strength associated with V_M is substantially larger than that of V_K . In addition, the relative importance of IFC disorder can also be estimated from the mismatch in elastic constants. Specifically, the strength of elastic scattering induced by IFC disorder is evaluated by the prefactor S_{el}^2 , with $S_{\text{el}} \sim [(\rho_s/\rho_m)v_s^2 - v_m^2]/v_m^2$, where ρ_m and ρ_s are the bulk densities of the matrix and solute species, and v_m and v_s denote their sound velocities, which can be taken for either longitudinal acoustic (LA) or transverse

acoustic (TA) modes [78]. For AlN and GaN, the bulk densities ρ are 3.271 and 6.040 g cm⁻³, respectively. With the transverse (6124.9 and 4090.9 m s⁻¹) and longitudinal (10 598.3 and 7108.5 m s⁻¹) sound velocities of AlN and GaN, respectively, the estimated prefactors are $S_{\text{el,TA}} \approx -0.18$ and $S_{\text{el,LA}} \approx -0.17$, in agreement with IFC-based comparison.

Notably, Eq. (18) reveals that the phonon-defect scattering rate depends explicitly on the squared perturbation matrix elements, and reduces to Tamura's expression [50] for elastic mass-disorder scattering [Eqs. (6)–(8)] when only the mass-related term V_M is considered. In this formulation, the disorder strength is quantified by the site-resolved mass-variance parameter $g(i)$. By analogy, an IFC-variance parameter can be introduced to characterize the strength of V_K :

$$g_K(i) = \sum_s f_s(i) [1 - a_{K,s}(i)]^2, \quad (22)$$

where $a_{K,s}(i)$ denotes the on-site IFCs associated with species s relative to the average value. On the basis of our calculations for $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$, the mass-variance parameters are $g_M^{\text{Al,Ga}} = 0.195$ and $g_M^{\text{N}} = 1.87 \times 10^{-5}$, while the

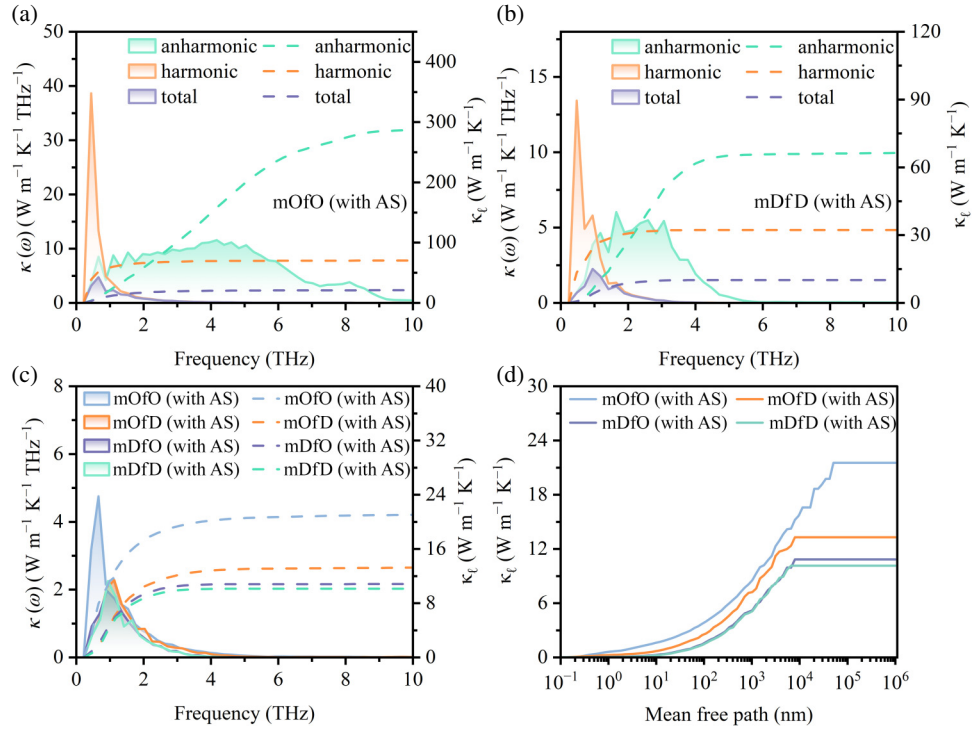


FIG. 8. Spectral and cumulative thermal conductivity of the $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$ disordered alloy at 300 K. (a),(b) Spectral and cumulative thermal conductivities calculated by inclusion of only harmonic (elastic) scattering or only anharmonic (phonon-phonon) scattering in comparison with the full calculation including both mechanisms. (c) Spectral and frequency cumulative thermal conductivity. (d) Mean free path cumulative thermal conductivity.

IFC-variance parameters are $g_K^{\text{Al,Ga}} = 0.00732$ and $g_K^{\text{N}} = 0.00631$. Overall, these results indicate that IFC disorder has a negligible impact compared with the dominant role of mass disorder.

A comparative analysis of phonon group velocities and scattering rates provides insights into the microscopic mechanisms underlying different types of disorder. As shown in Figs. 7(a)–7(c), the traditional VCA [mOfO (with AS)] approach significantly overestimates group velocities and underestimates scattering rates from low-frequency to mid-frequency phonons (0–5 THz), which dominate the heat conduction. In comparison, incorporation of IFC disorder [mOfD (with AS)] significantly increases anharmonic scattering rates. However, this modification has little effect on phonon group velocities and harmonic scattering rates, owing to the nearly unchanged phonon density of states in the low-frequency to mid-frequency range. Interestingly, mass disorder [mDfO (with AS)] simultaneously increases both harmonic and anharmonic scattering rates and suppresses phonon group velocities.

A more detailed examination of the scattering mechanisms reveals that different frequency ranges are dominated by distinct processes. Figure 7(d) shows that three-phonon anharmonic scattering dominates below 1 THz, while disorder-induced harmonic scattering prevails at

higher frequencies throughout the broad frequency spectrum. This shift in the dominant scattering mechanisms is further reflected in the spectral thermal conductivity, where harmonic scattering completely annihilates the heat-carrying ability of these higher-frequency phonons, as shown in Figs. 8(a) and 8(b). Notably, the incorporation of disorders simultaneously affects the contributions to the thermal conductivity in the low-frequency region (below 1 THz), thereby reducing the overall thermal conductivity [Figs. 8(a)–8(c)] of the system. This observation slightly differs from that of Garg *et al.* [18]. In $\text{Si}_x\text{Ge}_{1-x}$ alloys [18], mass disorder was found to affect only anharmonic scattering, while having a negligible effect on the thermal conductivity induced by harmonic scattering in the low-frequency region. The differences among mOfD (with AS), mDfO (with AS), and mDfD (with AS) arise mainly from phonon contributions within the 1–5 THz range.

Furthermore, cumulative thermal conductivity analysis indicates that phonons with mean free paths of less than 5 μm contribute more than 90% of the total thermal conductivity when disorder is included, suggesting that the system exhibits only minor sensitivity to sample size, as shown in Figs. 6(a) and 8(d). In contrast, earlier studies [8,14,16] attributed approximately 70% of the discrepancy

between theoretical predictions and experimental measurements to finite-size effects, while largely overlooking the impact of the random distribution of atomic masses and bonding environments in real disordered alloys on κ_ℓ . In line with these findings, recent vibrational studies [79] have shown that combined mass and IFC disorder can strongly reshape Raman spectra, highlighting the limitations of virtual-crystal and perturbative treatments. By explicitly accounting for both mass disorder and IFCs disorder, our results provide a more comprehensive and physically grounded explanation for the suppressed thermal conductivity in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys. Beyond bulk alloys, our findings may also be relevant to interfacial heat transport. In particular, if interfacial mixing leads to the formation of an $\text{Al}_x\text{Ga}_{1-x}\text{N}$ transition layer, disorder scattering could further suppress the phonons having a long mean free path and potentially alter the thickness dependence of thermal boundary conductance observed in GaN-AlN heterostructures [80].

Although incorporation of both mass disorder and IFC disorder leads to good agreement with experimental results, it should be noted that our current scattering rate calculations include only the elastic scattering term associated with mass disorder. However, the term for elastic scattering contributions [51] from IFC disorder is ignored in the total scattering rate expression, as discussed in Sec. II. The molecular dynamics method inherently includes all phonon-phonon scattering mechanisms, making it suitable for evaluating the impact of this omission on phonon scattering rates. Thus, we compared the phonon scattering rates obtained from the mDfD (with AS) and EMD methods to evaluate the impact of this omission, as shown in Fig. 6(b).

In the EMD method, the phonon lifetimes were calculated by our analyzing longitudinal and transverse current autocorrelation functions obtained from the EMD trajectories with the use of a damped harmonic oscillator model. The damping coefficient Γ , which is related to the phonon lifetime τ ($\tau = 2/\Gamma$) [81], is determined either by fitting the time-domain exponential decay profile or the frequency-domain Lorentzian peak. Both methods show good agreement of the computed scattering rates in the frequency range below 3 THz, which is considered to be the dominant heat carrier range and contributes more than 98% of the total κ_ℓ . This indicates that the mDfD (with AS) method can reliably predict thermal conductivity, as further supported by the excellent agreement between its predictions and HNEMD results across the entire range of Al content, as shown in Fig. 6(a). Nonetheless, it is worth noting that as the phonon frequency increases, the scattering rate calculated with the mDfD (with AS) method, which is based on perturbation theory, becomes progressively less reliable. For example, as shown in Fig. 6(b), this approach significantly overestimates the scattering of high-frequency optical phonons above 10 THz. It should

be noted that EMD is intrinsically based on classical statistics, whereas the BTE explicitly incorporates quantum Bose-Einstein statistics. In quantum statistics, the phonon occupation is described by the Bose-Einstein distribution $n(\omega, T) = 1/(e^{\hbar\omega/k_B T} - 1)$, which in the high-temperature limit reduces to the classical form $n(\omega, T) \approx k_B T/\hbar\omega$. To qualitatively assess the temperature range over which the classical approximation becomes valid, we compared the anharmonic three-phonon scattering rates obtained from the BTE at different temperatures with those obtained at 1000 K. As shown in Fig. S10 [48], the scattering rates at 300 K rescaled by $1000/T$ agree well with those at 1000 K, since the scattering channels are dominated by lower-frequency modes. This analysis indicates that phonon populations at room temperature are already close to the classical regime, thereby justifying a direct comparison between MD and BTE results at 300 K. In addition, we compared the total scattering rates obtained from EMD with the harmonic-only scattering rates predicted by the perturbation-based alloy scattering model, as displayed in the inset in Fig. 6(b). Because harmonic scattering is independent of quantum statistics and does not depend on temperature, it provides a natural reference. Nevertheless, the harmonic scattering rates are still significantly higher than the total scattering rates obtained from EMD in the high-frequency region.

Finally, it is worth noting that although the perturbation-based alloy scattering model that includes only mass-disorder scattering provides a satisfactory description for the present $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloy, where the mass-disorder perturbation is much stronger than the IFC-disorder perturbation, its applicability may not be generally transferable to alloy systems in which local force-constant variations dominate over mass fluctuations, for example, in alloys with a relatively small mass contrast but pronounced local bonding distortions, lattice-size mismatch, or chemical-environment variations, where IFC disorder can become comparable to or even more important than mass disorder. For such systems, the T -matrix formalism [76,77] provides a more general framework for treating alloy-induced elastic phonon scattering, because it can incorporate both mass and IFC perturbations through the full scattering operator, rather than considering only mass fluctuations as in the Tamura-type mass-disorder treatment [50]. Therefore, although the omitted elastic scattering associated with IFC disorder is expected to be small in the present $\text{Al}_x\text{Ga}_{1-x}\text{N}$ system and should not alter our conclusions, a direct comparison between the present perturbation-based framework and a full T -matrix approach would still be highly worthwhile, especially in the high-frequency region, where the phonon scattering rates obtained with the perturbative alloy scattering model deviate from the EMD results [Fig. 6(b)]. Such a comparison, however, is beyond the scope of the present work and will be an important topic for future study.

IV. CONCLUSION

In this study, we developed a high-fidelity NEP model for the $\text{Al}_x\text{Ga}_{1-x}\text{N}$ system via an active learning strategy. This model accurately reproduces key physical properties, including phonon dispersion, elastic constants, and κ_ℓ . Using this model, we systematically investigated how mass disorder and IFC disorder affect κ_ℓ of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys. The results show that the conventional VCA [mOfO (with AS)], which ignores local atomic variations, systematically overestimates κ_ℓ by 52%–131%. Incorporation of mass disorder [mDfO (with AS)] or IFC disorder [mOfD (with AS)] significantly reduced the prediction errors, while our combining both [mDfD (with AS)] yielded results that are in close agreement with the experimental measurements, highlighting the critical role of disorder in thermal transport. This importance is further supported by the substantial overestimation of κ_ℓ caused by artificial long-range periodicity in SQS-expanded supercells. Cumulative mean free path analysis shows that more than 90% of heat is carried by phonons with mean free paths shorter than 5 μm . This demonstrates that the long-standing VCA-experiment discrepancy stems from the ignoring of disorder scattering rather than finite-size effects. Frequency-domain analysis reveals that mass disorder predominantly suppresses thermal transport by reducing group velocities and increasing phonon scattering rates below 5 THz, whereas IFC disorder mainly increases the anharmonic scattering. Notably, the thermal transport of heat-carrying low-frequency phonons (below 1 THz), which contribute more than 50% of the total thermal conductivity, is limited primarily by anharmonic processes. The comparison between EMD and the mDfD (with AS) scheme shows good agreement below approximately 3 THz, supporting the reliability of our results. At higher frequencies (above 10 THz), the perturbation-based alloy model overestimates harmonic scattering, reflecting the limitation of the perturbative treatment for high-frequency modes.

This study provides significant theoretical insights as well as substantial guidance to mitigate heat accumulation in the near-junction regions of GaN-based high-power electronic devices and increase their thermal reliability. In these high-power-density HEMTs, inevitable alloy disorder in the barrier layer, buffer layer, and intermixing transition region reshapes the effective thermal resistance and redirects heat-flow pathways. The near-junction hot-spot temperature rise is strongly influenced by the composition profile, the degree of intermixing, and defect incorporation. Accordingly, disorder can be treated as a key controllable variable in device thermal design. Optimization of the transition-layer thickness and composition distribution through epitaxy and process control reduces the near-junction thermal resistance, while preserving the advantages in bandgap, polarization charge, and breakdown capability. More broadly, this work establishes

a transferable computational framework that goes beyond conventional VCA-based treatments by explicitly accounting for atomic-scale disorder, enabling more accurate thermal transport predictions in technologically important semiconductor alloys for energy-relevant applications. Future work could integrate high-fidelity MLP-driven thermal transport predictions with device-level electrothermal-mechanical-coupled modeling to establish a quantitative mapping from epitaxial parameters and interfacial intermixing to junction-temperature evolution and device lifetime, thereby enabling predictive design rules for thermal management in wide-bandgap power electronics.

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Yuwen Zhang wrote the original draft, conducted the investigation, curated the data, and prepared the visualizations. Tao Ouyang provided resources and contributed to the software. Zheyong Fan contributed to the software and performed the formal analysis. Wu Li conceptualized the study, acquired funding, and reviewed and edited the manuscript.

The authors declare that they have no conflicts of interest.

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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- [1] J. Piprek, Ultra-violet light-emitting diodes with quasi acceptor-free AlGaIn polarization doping, *Opt. Quantum Electron.* **44**, 67 (2012).
 - [2] C.-P. Wang and Y.-R. Wu, Study of optical anisotropy in nonpolar and semipolar AlGaIn quantum well deep ultra-violet light emission diode, *J. Appl. Phys.* **112**, 033104 (2012).
 - [3] I. Omura, W. Saito, T. Domon, and K. Tsuda, Gallium Nitride power HEMT for high switching frequency power electronics, in *2007 International Workshop on Physics of Semiconductor Devices* (2007), p. 781.
 - [4] A. S. A. Fletcher and D. Nirmal, A survey of gallium nitride HEMT for RF and high power applications, *Superlattices. Microstruct.* **109**, 519 (2017).
 - [5] J. Zhang and N. Tansu, Engineering of AlGaIn-Delta-GaN quantum-well gain media for mid- and deep-ultraviolet lasers, *IEEE Photonics J.* **5**, 2600209 (2013).

- [6] S. Ali and M. Usman, Performance enhancement of ultraviolet-C AlGaIn laser diode, *Eur. Phys. J. Plus* **137**, 771 (2022).
- [7] A. G. Baca, A. M. Armstrong, B. A. Klein, A. A. Allerman, E. A. Douglas, and R. J. Kaplar, Al-rich AlGaIn based transistors, *J. Vac. Sci. Technol. A* **38**, 020803 (2020).
- [8] D. Q. Tran, R. D. Carrascon, M. Iwaya, B. Monemar, V. Darakchieva, and P. P. Paskov, Thermal conductivity of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ ($0 \leq x \leq 1$) epitaxial layers, *Phys. Rev. Mater.* **6**, 104602 (2022).
- [9] T.-L. Luo, Y.-F. Ding, B.-J. Wei, J.-Y. Du, X.-Y. Shen, G.-M. Zhu, and B.-W. Li, Phononic thermal conduction and thermal regulation in low-dimensional micro-nano scale systems: Nonequilibrium statistical physics problems from chip heat dissipation, *Acta Phys. Sin.* **72**, 234401 (2023).
- [10] Z. Qi, W. Shen, R. Li, X. Sun, L. Li, Q. Wang, G. Wu, and K. Liang, AlN/diamond interface nanoengineering for reducing thermal boundary resistance by molecular dynamics simulations, *Appl. Surf. Sci.* **615**, 156419 (2023).
- [11] A. Chen, D. Wei, J. Xu, A. Li, H. Wang, Z. Qin, and G. Qin, Alloying reversed anisotropy of thermal transport in bulk $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$, *J. Phys. Chem. Lett.* **14**, 9746 (2023).
- [12] W. Liu and A. A. Balandin, Temperature dependence of thermal conductivity of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ thin films measured by the differential 3ω technique, *Appl. Phys. Lett.* **85**, 5230 (2004).
- [13] W. Liu and A. A. Balandin, Thermal conduction in $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys and thin films, *J. Appl. Phys.* **97**, 073710 (2005).
- [14] D. Q. Tran, R. Delgado-Carrascon, J. F. Muth, T. Paskova, M. Nawaz, V. Darakchieva, and P. P. Paskov, Phonon-boundary scattering and thermal transport in $\text{Al}_x\text{Ga}_{1-x}\text{N}$: Effect of layer thickness, *Appl. Phys. Lett.* **117**, 252102 (2020).
- [15] D. G. Cahill, Thermal conductivity measurement from 30 to 750 K: The 3ω method, *Rev. Sci. Instrum.* **61**, 802 (1990).
- [16] J. Ma, W. Li, and X. Luo, Intrinsic thermal conductivities and size effect of alloys of wurtzite AlN, GaN, and InN from first-principles, *J. Appl. Phys.* **119**, 125702 (2016).
- [17] B. Abeles, Lattice thermal conductivity of disordered semiconductor alloys at high temperatures, *Phys. Rev.* **131**, 1906 (1963).
- [18] J. Garg, N. Bonini, B. Kozinsky, and N. Marzari, Role of disorder and anharmonicity in the thermal conductivity of silicon-germanium alloys: A first-principles study, *Phys. Rev. Lett.* **106**, 045901 (2011).
- [19] T. Dao-Sheng, H. Yu-Chao, Z. Yan-Guang, and C. Bing-Yang, Thermal conductivity modeling of GaN films, *Acta Phys. Sin.* **70**, 045101 (2021).
- [20] G. Yang, Y.-B. Liu, L. Yang, and B.-Y. Cao, Machine-learned atomic cluster expansion potentials for fast and quantum-accurate thermal simulations of wurtzite AlN, *J. Appl. Phys.* **135**, 085105 (2024).
- [21] A. Ward, D. A. Broido, D. A. Stewart, and G. Deinzer, Ab initio theory of the lattice thermal conductivity in diamond, *Phys. Rev. B* **80**, 125203 (2009).
- [22] R. Drautz, Atomic cluster expansion for accurate and transferable interatomic potentials, *Phys. Rev. B* **99**, 014104 (2019).
- [23] Z. Fan, Y. Wang, P. Ying, K. Song, J. Wang, Y. Wang, Z. Zeng, K. Xu, E. Lindgren, J. M. Rahm, A. J. Gabourie, J. Liu, H. Dong, J. Wu, Y. Chen, Z. Zhong, J. Sun, P. Erhart, Y. Su, and T. Ala-Nissila, GPUMD: A package for constructing accurate machine-learned potentials and performing highly efficient atomistic simulations, *J. Chem. Phys.* **157**, 114801 (2022).
- [24] Z. Fan, Z. Zeng, C. Zhang, Y. Wang, K. Song, H. Dong, Y. Chen, and T. Ala-Nissila, Neuroevolution machine learning potentials: Combining high accuracy and low cost in atomistic simulations and application to heat transport, *Phys. Rev. B* **104**, 104309 (2021).
- [25] Z. Fan, Improving the accuracy of the neuroevolution machine learning potential for multi-component systems, *J. Phys.: Condens. Matter* **34**, 125902 (2022).
- [26] L. Dai, M. Li, and Y. Hu, Machine learning for thermal transport and phonon high-order anharmonicity in high thermal conductivity materials: A case study in boron arsenide, *Phys. Rev. Mater.* **9**, 045403 (2025).
- [27] I. S. Novikov, K. Gubaev, E. V. Podryabinkin, and A. V. Shapeev, The MLIP package: Moment tensor potentials with MPI and active learning, *Mach. Learn.: Sci. Technol.* **2**, 025002 (2021).
- [28] J. Tiwari and T. Feng, Accurate prediction of thermal conductivity of Al_2O_3 at ultrahigh temperatures, *Phys. Rev. B* **109**, 075201 (2024).
- [29] L. Zhang, J. Han, H. Wang, R. Car, and W. E, Deep potential molecular dynamics: A scalable model with the accuracy of quantum mechanics, *Phys. Rev. Lett.* **120**, 143001 (2018).
- [30] H. Dong, Z. Li, B. Sun, Y. Zhou, L. Liu, and J.-Y. Yang, Thermal transport in disordered wurtzite ScAlN alloys using machine learning interatomic potentials, *Mater. Today Commun.* **39**, 109213 (2024).
- [31] Z. Sun, X. Sun, Z. Qi, Q. Wang, R. Li, L. Li, G. Wu, W. Shen, and S. Liu, Investigating thermal transport across the AlN/diamond interface via the machine learning potential, *Diamond Relat. Mater.* **147**, 111303 (2024).
- [32] K. Song *et al.*, General-purpose machine-learned potential for 16 elemental metals and their alloys, *Nat. Commun.* **15**, 10208 (2024).
- [33] G. Kresse and J. Furthmüller, Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set, *Phys. Rev. B* **54**, 11169 (1996).
- [34] P. E. Blöchl, Projector augmented-wave method, *Phys. Rev. B* **50**, 17953 (1994).
- [35] G. Kresse and D. Joubert, From ultrasoft pseudopotentials to the projector augmented-wave method, *Phys. Rev. B* **59**, 1758 (1999).
- [36] J. P. Perdew, K. Burke, and M. Ernzerhof, Generalized gradient approximation made simple, *Phys. Rev. Lett.* **77**, 3865 (1996).
- [37] H. J. Monkhorst and J. D. Pack, Special points for Brillouin-zone integrations, *Phys. Rev. B* **13**, 5188 (1976).
- [38] X. Z. Shi, C. Y. He, C. J. Pickard, C. Tang, and J. X. Zhong, Stochastic generation of complex crystal structures combining group and graph theory with application to carbon, *Phys. Rev. B* **97**, 014104 (2018).
- [39] A. Jain, S. P. Ong, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder, and K. A. Persson, Commentary: The Materials Project: A materials genome approach to accelerating materials innovation, *APL Mater.* **1**, 011002 (2013).

- [40] W. Li, J. Carrete, N. A. Katcho, and N. Mingo, ShengBTE: A solver of the Boltzmann transport equation for phonons, *Comput. Phys. Commun.* **185**, 1747 (2014).
- [41] Z. Han, X. Yang, W. Li, T. Feng, and X. Ruan, FourPhonon: An extension module to ShengBTE for computing four-phonon scattering rates and thermal conductivity, *Comput. Phys. Commun.* **270**, 108179 (2022).
- [42] S. Grimme, J. Antony, S. Ehrlich, and H. Krieg, A consistent and accurate *ab initio* parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu, *J. Chem. Phys.* **132**, 154104 (2010).
- [43] S. Grimme, S. Ehrlich, and L. Goerigk, Effect of the damping function in dispersion corrected density functional theory, *J. Comput. Chem.* **32**, 1456 (2011).
- [44] A. Togo and I. Tanaka, First principles phonon calculations in materials science, *Scr. Mater.* **108**, 1 (2015).
- [45] A. Szein, J. Haberstroh, J. E. Bowers, S. P. DenBaars, and S. Nakamura, Calculated thermoelectric properties of $\text{In}_x\text{Ga}_{1-x}\text{N}$, $\text{In}_x\text{Al}_{1-x}\text{N}$, and $\text{Al}_x\text{Ga}_{1-x}\text{N}$, *J. Appl. Phys.* **113**, 183707 (2013).
- [46] A. Zunger, S. H. Wei, L. G. Ferreira, and J. E. Bernard, Special quasirandom structures, *Phys. Rev. Lett.* **65**, 353 (1990).
- [47] M. Ångqvist, W. A. Muñoz, J. M. Rahm, E. Fransson, C. Durniak, P. Rozyczko, T. H. Rod, and P. Erhart, ICET – A Python library for constructing and sampling alloy cluster expansions, *Adv. Theory Simul.* **2**, 1900015 (2019).
- [48] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/df1n-9bll> for additional results and validations, including convergence tests of lattice thermal conductivity with respect to $\mathbf{q}$ -point sampling, supercell size, and the sampling method; validation of the NEP model against DFT for crystalline phases, heterostructures, and out-of-sample alloy compositions; representative SQS configurations of $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys used in this work; and a comparison of anharmonic scattering rates of the $\text{Al}_{0.5}\text{Ga}_{0.5}\text{N}$ alloy at different temperatures.
- [49] W. Li, L. Lindsay, D. A. Broido, D. A. Stewart, and N. Mingo, Thermal conductivity of bulk and nanowire $\text{Mg}_2\text{Si}_x\text{Sn}_{1-x}$ alloys from first principles, *Phys. Rev. B* **86**, 174307 (2012).
- [50] S.-I. Tamura, Isotope scattering of dispersive phonons in Ge, *Phys. Rev. B* **27**, 858 (1983).
- [51] A. Katre, J. Carrete, B. Dongre, G. K. H. Madsen, and N. Mingo, Exceptionally strong phonon scattering by B substitution in cubic SiC, *Phys. Rev. Lett.* **119**, 075902 (2017).
- [52] Z. Fan, H. Dong, A. Harju, and T. Ala-Nissila, Homogeneous nonequilibrium molecular dynamics method for heat transport and spectral decomposition with many-body potentials, *Phys. Rev. B* **99**, 064308 (2019).
- [53] D. J. Evans, Homogeneous nemd algorithm for thermal conductivity—Application of non-canonical linear response theory, *Phys. Lett. A* **91**, 457 (1982).
- [54] K. K. Mandadapu, R. E. Jones, and P. Papadopoulos, A homogeneous nonequilibrium molecular dynamics method for calculating thermal conductivity with a three-body potential, *J. Chem. Phys.* **130**, 204106 (2009).
- [55] T. Ruf, J. Serrano, M. Cardona, P. Pavone, M. Pabst, M. Krisch, M. D'Astuto, T. Suski, I. Grzegory, and M. Leszczynski, Phonon dispersion curves in wurtzite-structure GaN determined by inelastic X-ray scattering, *Phys. Rev. Lett.* **86**, 906 (2001).
- [56] M. Schwoerer-Böhning, A. T. Macrander, M. Pabst, and P. Pavone, Phonons in wurtzite aluminum nitride, *Phys. Status Solidi (b)* **215**, 177 (1999).
- [57] J. M. Zhang, T. Ruf, M. Cardona, O. Ambacher, M. Stutzmann, J. M. Wagner, and F. Bechstedt, Raman spectra of isotopic GaN, *Phys. Rev. B* **56**, 14399 (1997).
- [58] Z. Cheng, Y. R. Koh, A. Mamun, J. Shi, T. Bai, K. Huynh, L. Yates, Z. Liu, R. Li, E. Lee, M. E. Liao, Y. Wang, H. M. Yu, M. Kushimoto, T. Luo, M. S. Goorsky, P. E. Hopkins, H. Amano, A. Khan, and S. Graham, Experimental observation of high intrinsic thermal conductivity of AlN, *Phys. Rev. Mater.* **4**, 044602 (2020).
- [59] A. V. Inyushkin, A. N. Taldenkov, D. A. Chernodubov, E. N. Mokhov, S. S. Nagalyuk, V. G. Ralchenko, and A. A. Khomich, On the thermal conductivity of single crystal AlN, *J. Appl. Phys.* **127**, 205109 (2020).
- [60] L. Lindsay, D. A. Broido, and T. L. Reinecke, Thermal conductivity and large isotope effect in GaN from first principles, *Phys. Rev. Lett.* **109**, 095901 (2012).
- [61] G. A. Slack, R. A. Tanzilli, R. O. Pohl, and J. W. Vanderlande, The intrinsic thermal conductivity of AlN, *J. Phys. Chem. Solids* **48**, 641 (1987).
- [62] Q. Zheng, C. Li, A. Rai, J. H. Leach, D. A. Broido, and D. G. Cahill, Thermal conductivity of GaN, ^{71}GaN , and SiC from 150 K to 850 K, *Phys. Rev. Mater.* **3**, 014601 (2019).
- [63] H. Shibata, Y. Waseda, H. Ohta, K. Kiyomi, K. Shimoyama, K. Fujito, H. Nagaoka, Y. Kagamitani, R. Simura, and T. Fukuda, High thermal conductivity of gallium nitride (GaN) crystals grown by HVPE process, *Mater. Trans.* **48**, 2782 (2007).
- [64] L. Lindsay, D. A. Broido, and T. L. Reinecke, Ab initio thermal transport in compound semiconductors, *Phys. Rev. B* **87**, 165201 (2013).
- [65] W. Li and N. Mingo, Thermal conductivity of bulk and nanowire InAs, AlN, and BeO polymorphs from first principles, *J. Appl. Phys.* **114**, 183505 (2013).
- [66] R. Wu, R. Hu, and X. Luo, First-principle-based full-dispersion Monte Carlo simulation of the anisotropic phonon transport in the wurtzite GaN thin film, *J. Appl. Phys.* **119**, 145706 (2016).
- [67] J. Garg, T. Luo, and G. Chen, Spectral concentration of thermal conductivity in GaN—A first-principles study, *Appl. Phys. Lett.* **112**, 252101 (2018).
- [68] B. C. Daly, H. J. Maris, A. V. Nurmikko, M. Kuball, and J. Han, Optical pump-and-probe measurement of the thermal conductivity of nitride thin films, *J. Appl. Phys.* **92**, 3820 (2002).
- [69] A. Filatova-Zalewska, Z. Litwicki, T. Suski, and A. Jeżowski, Thermal conductivity of thin films of gallium nitride, doped with aluminium, measured with 3ω method, *Solid State Sci.* **101**, 106105 (2020).
- [70] P. F. de Aguiar, B. Bourguignon, M. S. Khots, D. L. Massart, and R. Phan-Than-Luu, D-optimal designs, *Chemometr. Intell. Lab. Syst.* **30**, 199 (1995).
- [71] E. Podryabinkin, K. Garifullin, A. Shapeev, and I. Novikov, MLIP-3: Active learning on atomic environments with

- moment tensor potentials, *J. Chem. Phys.* **159**, 084112 (2023).
- [72] S. A. Goreinov, I. V. Oseledets, D. V. Savostyanov, E. E. Tyrtyshnikov, and N. L. Zamarashkin, How to find a good submatrix, in *Matrix Methods: Theory, Algorithms and Applications* (World Scientific, Singapore, 2010), p. 247.
- [73] https://github.com/psn417/nep_extrapolation.
- [74] L. Zhang, H. Yan, G. Zhu, S. Liu, Z. Gan, and Z. Zhang, Effect of substrate surface on deposition of AlGaIn: A molecular dynamics simulation, *Crystals* **8**, 279 (2018).
- [75] D.-S. Tang and B.-Y. Cao, Phonon thermal transport and its tunability in GaN for near-junction thermal management of electronics: A review, *Int. J. Heat Mass Transf.* **200**, 123497 (2023).
- [76] A. Katre, J. Carrete, B. Dongre, G. K. H. Madsen, and N. Mingo, Exceptionally strong phonon scattering by B substitution in cubic SiC, *Phys. Rev. Lett.* **119**, 075902 (2017).
- [77] G. Pang, F. Meng, Y. Chen, A. Katre, J. Carrete, B. Dongre, G. K. Madsen, N. Mingo, and W. Li, Thermal conductivity reduction in highly-doped cubic SiC by phonon-defect and phonon-electron scattering, *Mater. Today Phys.* **41**, 101346 (2024).
- [78] A. Kundu, N. Mingo, D. A. Broido, and D. A. Stewart, Role of light and heavy embedded nanoparticles on the thermal conductivity of SiGe alloys, *Phys. Rev. B* **84**, 125426 (2011).
- [79] H. Wu, Z. Qin, S. Li, L. Lindsay, and Y. Hu, Non-perturbative determination of isotope-induced anomalous vibrational physics, *Phys. Rev. B* **108**, L140302 (2023).
- [80] M. Li, K. Pan, Y. Ge, K. Huynh, M. S. Goorsky, T. S. Fisher, and Y. Hu, Wafer-scale bonded GaN–AlN with high interface thermal conductance, *Appl. Phys. Lett.* **125**, 032104 (2024).
- [81] E. Fransson, M. Slabanja, P. Erhart, and G. Wahnström, Dynasor—A tool for extracting dynamical structure factors and current correlation functions from molecular dynamics simulations, *Adv. Theory Simul.* **4**, 2000240 (2021).