

First-principles electronic transport properties of Ti and Ti-6Al-4V for modeling ultrashort-pulse laser ablation

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Predictive modeling of ultrashort-pulse laser ablation requires temperature-dependent material parameters derived from the electronic structure, namely the electronic thermal conductivity, electron-phonon coupling, and heat capacity. These parameters are well documented for elemental metals but remain sparsely documented for alloys, apart from application-relevant exceptions such as stainless steels. The technologically important titanium alloy Ti-6Al-4V is a prominent example, which is still modeled using elemental-titanium values. We compute the electronic transport of hcp Ti and Ti-6Al-4V from first principles, using the Kubo-Greenwood formalism within the Korringa-Kohn-Rostoker coherent-potential-approximation framework, treating chemical and thermal disorder on equal footing. For elemental Ti, the calculated electrical resistivity agrees with independent ABINIT electron-phonon calculations and experiment and also reproduces the high-temperature saturation near the Mott-Ioffe-Regel limit. Under electron-phonon nonequilibrium, the electronic thermal conductivity saturates and then decreases with electronic temperature, reaching a maximum of about $2.97 \text{ kW m}^{-1} \text{ K}^{-1}$ in Ti but only $0.47 \text{ kW m}^{-1} \text{ K}^{-1}$ in Ti-6Al-4V, a factor of 6.4 lower. In two-temperature-model simulations the alloy and elemental parameter sets yield peak lattice temperatures differing by only about 1.4%, because reduced electron-phonon coupling and thermal conductivity offset each other, consistent with reported experimental ablation thresholds that differ by about 3%, well within their measurement uncertainties. This compensation is strongest for subpicosecond pulses and weakens across the 1 to 10 ps crossover toward longer-pulse behavior. Replacing the first-principles thermal conductivity with the low-temperature Drude limit shifts the peak lattice temperature by up to 19%, showing that the functional form of the transport model is even more important than the elemental versus alloy distinction for predictive accuracy.

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I. INTRODUCTION

Ti-6Al-4V (grade 5 titanium) is the workhorse of titanium applications in medicine, science, and industry, valued for its high strength-to-weight ratio, corrosion resistance, biocompatibility, and thermal stability [1,2], which makes it central to, e.g., lightweight aerospace design and to orthopedic and dental implants [3–6]. These applications place strict requirements on machining precision and surface texture, for which laser processing has become a key enabling

technology. Ultrashort-pulse (USP) lasers enable micrometer-scale machining and submicrometer functional surface textures that improve wettability, osseointegration, and cellular response [7–11].

For pulse durations shorter than the electron-phonon equilibration time (in the picosecond range), predictive modeling relies on the two-temperature model (TTM) [12], which couples electronic and lattice subsystems through Fourier heat equations, linked by electron-phonon energy transfer [13,14]. The TTM for metals and alloys is based on four electron (T_e) and lattice (T_l) temperature-dependent material parameters, namely the electronic and lattice heat capacities C_e and C_l , the electronic thermal conductivity κ_e , and the electron-phonon coupling factor G . The lattice thermal conductivity, which scales as $1/T_l$ and remains smaller than the electronic conductivity, is typically disregarded for metals and alloys.

For pure metals these parameters are well documented. Lin *et al.* provided an electron-temperature-dependent description of the electron-phonon coupling G from the

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electronic density of states [15]. The electron thermal conductivity is usually captured by the low-temperature Drude limit, $\kappa_e = \kappa_{e0} T_e/T_1$ [13], where κ_{e0} is the electronic thermal conductivity at room temperature or by more complex models [16]. For alloys, however, the data are far more sparse. Winter *et al.* [17] and Bévilion *et al.* [18] extended the density-of-states-based C_e and G description to stainless steel, and first-principles studies have addressed the equilibrium electronic transport of concentrated solid solutions [19,20]. The electronic thermal conductivity under electron-phonon nonequilibrium, by contrast, remains largely undetermined apart from a few exceptions [21] and especially so for Ti-6Al-4V. Most USP ablation simulations of Ti-6Al-4V therefore default to elemental-titanium parameters, in particular for κ_e and G [22–25].

In the present work we address these gaps. The electronic structure and transport properties of the hexagonal phases of Ti and Ti-6Al-4V are computed as functions of both T_e and T_1 within the Korringa-Kohn-Rostoker (KKR) Green's function formalism [26], treating chemical disorder by the coherent potential approximation (CPA) and thermal disorder by the alloy-analogy model on the same footing. For elemental Ti, the resistivity obtained from the Kubo-Greenwood linear-response framework [27] is cross-checked against independent ABINIT electron-phonon calculations [28]. The heat capacity C_e , the coupling factor G , and, in particular, κ_e under electron-phonon nonequilibrium are then computed for both Ti and the alloy. These properties feed one-dimensional TTM simulations, in which the full first-principles parameters are compared with the approximations commonly used for elemental Ti and with the corresponding Ti-6Al-4V values. Finally, a sensitivity analysis quantifies how each parameter influences the prediction of the ablation threshold as a function of pulse duration.

II. METHODS

A. Electronic structure calculations

Electronic-structure calculations for Ti and Ti-6Al-4V were performed within the fully relativistic KKR Green-function formalism as implemented in the spin-polarized relativistic Korringa-Kohn-Rostoker (SPR-KKR) package [26,29]. Exchange and correlation were described within the generalized gradient approximation (GGA) in the Perdew-Burke-Ernzerhof (PBE) parametrization [30], following systematic benchmarks of PBE for solids [31] and previous GGA studies of Ti [32] and Ti-6Al-4V [33]. The angular-momentum expansion of the Green function was truncated after f -character contributions, and Brillouin-zone (BZ) integrations employed a $60 \times 60 \times 33$ k -point mesh for the hexagonal lattice.

For Ti-6Al-4V, substitutional chemical disorder among Ti, Al, and V was treated within the CPA, in which each site carries the average occupation with atomic fractions $x_{\text{Ti}} = 0.862$, $x_{\text{Al}} = 0.102$, and $x_{\text{V}} = 0.036$, corresponding to the nominal composition of 6 wt.% Al and 4 wt.% V. The Ti-6Al-4V results should therefore be understood as an idealized, substitutionally disordered reference alloy. Room-temperature lattice parameters of the hexagonal close-packed (hcp) struc-

TABLE I. Structural and thermal input parameters. The lattice constants are room-temperature values, averaged over the references cited for pure Ti [34–36] and for Ti-6Al-4V [35,37–39]. The mechanical Debye temperature Θ_D^{mech} , taken from Ref. [45] and used for both Ti and Ti-6Al-4V [46], enters the alloy-analogy-model (AAM) thermal-displacement calculation, whereas the effective thermodynamic Debye temperature Θ_D^{th} enters the electron-phonon coupling G and the lattice heat capacity C_l (see the Supplemental Material [41]).

System	a (Å)	c (Å)	Θ_D^{mech} (K)	Θ_D^{th} (K)
Ti	2.95	4.68	385	415
Ti-6Al-4V	2.93	4.68	385	415

ture were obtained by averaging the experimental values reported in Refs. [34–36] for Ti and Refs. [35,37–39] for Ti-6Al-4V. The resulting in-plane a and out-of-plane c are listed in Table I.

Lattice thermal disorder was incorporated through the alloy-analogy model (AAM) [40], in which thermally displaced atomic configurations are mapped onto an effective substitutional alloy. The displaced-alloy components were generated from a symmetry-adapted cluster construction that respects the crystal symmetry, with 18 isotropic directions, and the displacement distribution was taken to be isotropic. Test calculations using molecular-dynamics and first-principles data showed only negligible anisotropy (below 5% relative difference in the mean-square atomic displacement) over the temperature range relevant here (see Supplemental Material [41]). The molecular-dynamics reference data were generated with LAMMPS [42] using the interatomic potential of Hennig *et al.* [43].

The temperature-dependent mean-square displacement was obtained from the Debye model [44],

$$\langle u^2 \rangle = \frac{9\hbar^2}{k_B \Theta_D^{\text{mech}} M} \left[\frac{1}{4} + \left(\frac{T}{\Theta_D^{\text{mech}}} \right)^2 \int_0^{\Theta_D^{\text{mech}}/T} \frac{t}{e^t - 1} dt \right], \quad (1)$$

where M is the mean atomic mass, Θ_D^{mech} the mechanical Debye temperature, k_B the Boltzmann constant, $\hbar$ the reduced Planck constant, and T the lattice temperature. The value $\Theta_D^{\text{mech}} = 385$ K was taken from Ref. [45] and used for both Ti and Ti-6Al-4V, since the hcp-phase Debye temperature reported for the alloy is nearly identical [46]. The zero-point contribution was omitted following Ref. [40]. First-principles calculations performed with the ABINIT package (see Sec. II B) yielded a consistent value of 360 K (see Supplemental Material [41]). The corresponding structural and thermal input parameters are summarized in Table I.

Initial tests showed that thermal expansion [47] and self-consistent displaced potentials change the temperature-dependent resistivity only marginally (see the Supplemental Material [41]). All subsequent calculations were therefore carried out with the experimental lattice parameters of Table I and with the self-consistent potential of the corresponding undistorted structure. Finite electronic temperature was considered in the subsequent transport and thermodynamic quantities through the Fermi occupations and the

temperature-dependent chemical potential, while the underlying self-consistent potential was not recalculated at finite electronic temperature. Apart from a chemical-potential shift the density-of-states (DOS) shape changes only marginally over the relevant range, as verified with the full-potential linearized augmented-plane-wave code ELK [48] (see the Supplemental Material [41]).

B. Electronic transport properties

Electronic transport was evaluated within the Kubo-Greenwood (KG) linear-response formalism as implemented in SPR-KKR [26,27]. The energy-resolved conductivity tensor is

$$\sigma_{\mu\nu}(E) = \frac{\hbar}{\pi N \Omega} \text{Tr} \left(\hat{j}_\mu \text{Im} G^+(E) \hat{j}_\nu \text{Im} G^+(E) \right)_c, \quad (2)$$

where E is the electron energy, N is the number of atomic sites, Ω the unit-cell volume, μ and ν denote Cartesian directions, $\hat{j}_\mu$ is the μ component of the relativistic current-density operator, $G^+(E)$ the retarded single-particle Green function, and $\langle \dots \rangle_c$ the CPA configurational average, including vertex corrections [26]. Equation (2) retains only the Fermi-surface term of the full Kubo-Bastin conductivity [49], and the electronic-temperature dependence enters solely through the Fermi-Dirac occupation in Eq. (3).

The full BZ was sampled with a $56 \times 56 \times 30$ $\mathbf{k}$ -point mesh after convergence tests (see the Supplemental Material [41]). All transport results reported below were obtained by including angular momentum components up to f orbitals. The dependence on the angular-momentum cutoff and on the exchange-correlation functional (local density approximation [50] versus GGA) is documented in the Supplemental Material [41].

In this scheme, the lattice temperature T_l enters through the AAM and the electronic temperature T_e through the Fermi-Dirac occupations in the transport integrals. The energy-resolved conductivity $\sigma_{\mu\nu}(E)$ was computed for a discrete set of lattice temperatures up to $T_l = 2100$ K and then linearly extrapolated to $T_l = 2500$ K ($\approx 1.3 T_m$, where T_m denotes the melting temperature). At each T_l , the energy grid covered the interval $\pm 6 k_B T_{e,\text{max}}$ around the Fermi level with 50 sampling points, where $T_{e,\text{max}} = 50$ kK. The electronic thermal conductivity was then obtained from the generalized (Onsager) transport coefficients (GTC) [19,51,52],

$$L_{ij}^{\mu\mu} = (-1)^{i+j} \int_{-\infty}^{\infty} dE \sigma_{\mu\mu}(E) (E - \mu_c)^{i+j-2} \left(-\frac{\partial f}{\partial E} \right), \quad (3)$$

where $f \equiv f(E, \mu_c, T_e)$ is the Fermi-Dirac distribution at electronic temperature T_e and $\mu_c(T_e)$ is the T_e -dependent chemical potential calculated from charge conservation of total valence-electron count from the DOS [17]. The longitudinal electronic thermal conductivity follows as

$$\kappa_{\mu\mu}(T_e, T_l) = \frac{1}{e^2 T_e} \left(L_{22}^{\mu\mu} - \frac{L_{12}^{\mu\mu} L_{21}^{\mu\mu}}{L_{11}^{\mu\mu}} \right). \quad (4)$$

As an independent benchmark, the electrical resistivity of hcp Ti was computed with the electron-phonon coupling module of ABINIT version 10.5.8 [28] by solving the iterative Boltzmann transport equation [53]. Fully rel-

ativistic norm-conserving PBE pseudopotentials from the PseudoDojo library [54], including spin-orbit coupling, were employed. The plane-wave cutoff was set to 40 Ha, with a Γ -centered $10 \times 10 \times 10$ $\mathbf{k}$ -point grid and a $5 \times 5 \times 5$ $\mathbf{q}$ -point grid for the phonon perturbations. Although the SPR-KKR calculations used the experimental lattice parameters of Table I, the ABINIT reference cell was fully relaxed, yielding $a = 2.943$ Å and $c = 4.640$ Å (residual stresses below 6×10^{-3} GPa). An energy window of 0.4 eV around the Fermi level and an interpolated $40 \times 40 \times 40$ $\mathbf{q}$ -point grid were used for the scattering potentials. Full methodological details are given in Refs. [55–57].

C. Two-temperature model

The thermal response to USP laser irradiation was modeled with a one-dimensional TTM [12], initialized at $T_e = T_l = 300$ K. Under stress confinement, USP laser ablation proceeds through photomechanical spallation and, at higher fluence, phase explosion [58,59]. Mechanical and hydrodynamic response as well as phase change are not considered. The peak lattice temperature reached during the simulation serves as a proxy for the ablation threshold, as it sets the deposited energy and the associated buildup of thermoelastic stress that drives material removal. The coupled energy-balance equations for the electronic and lattice subsystems read

$$C_e(T_e) \frac{\partial T_e}{\partial t} = \frac{\partial}{\partial z} \left[\kappa_e(T_e, T_l) \frac{\partial T_e}{\partial z} \right] - G(T_e) (T_e - T_l) + S(z, t), \quad (5)$$

$$C_l(T_l) \frac{\partial T_l}{\partial t} = \frac{\partial}{\partial z} \left[\kappa_l(T_l) \frac{\partial T_l}{\partial z} \right] + G(T_e) (T_e - T_l), \quad (6)$$

where z is the depth coordinate normal to a laser irradiated surface.

The laser source term was modeled as a Gaussian temporal pulse with Beer-Lambert linear absorption in z dimension,

$$S(z, t) = \frac{(1-R)F}{d_{\text{opt}}} \sqrt{\frac{4 \ln 2}{\pi \tau_p^2}} \times \exp\left(-\frac{z}{d_{\text{opt}}}\right) \exp\left(-4 \ln 2 \frac{(t - t_0)^2}{\tau_p^2}\right), \quad (7)$$

where F is the incident peak fluence, R the normal-incidence reflectance, d_{opt} the optical penetration depth at $\lambda_L = 1030$ nm, and $\tau_p = 300$ fs the temporal full width at half maximum of the pulse intensity. The optical constants were taken identical for Ti and Ti-6Al-4V, with $R = 0.614$ and $d_{\text{opt}} = 20.4$ nm, computed from the extinction coefficient $k = 3.99$ via $d_{\text{opt}} = \lambda/(4\pi k)$ [60]. Transient changes of the optical constants during the pulse were neglected, as the reflectivity of metals remains approximately constant up to the ablation threshold fluence [61].

The electronic heat capacity was computed from the self-consistent DOS, $n(E)$, according to

$$C_e(T_e) = \int_{-\infty}^{\infty} dE (E - \mu_c) \frac{\partial f(E, \mu_c, T_e)}{\partial T_e} n(E), \quad (8)$$

with the chemical potential $\mu_c(T_e)$ fixed by the same valence-electron conservation as in Eq. (3). The electron-phonon

coupling factor was evaluated following the formalism of Lin *et al.* [15],

$$G(T_e) = \frac{\pi \hbar k_B \lambda \langle \omega^2 \rangle}{n(E_F)} \int_{-\infty}^{\infty} dE n^2(E) \left(-\frac{\partial f}{\partial E} \right), \quad (9)$$

where $n(E_F)$ is the DOS at the Fermi level. The product $\lambda \langle \omega^2 \rangle$ is defined through the Eliashberg spectral function [62] as $\lambda \langle \omega^2 \rangle = 2 \int_0^{\infty} d\omega \alpha^2 F(\omega) \omega$. Approximating $\alpha^2 F(\omega)$ by a Debye spectrum with frequency-independent electron-phonon matrix elements yields $\langle \omega^2 \rangle = \frac{1}{2} (k_B \Theta_D^{\text{th}} / \hbar)^2$, evaluated with the thermodynamic Debye temperature Θ_D^{th} of Table I, following Lin *et al.* [15]. The electron-phonon coupling constants λ are taken from Ref. [63]. For Ti-6Al-4V, effective values were constructed from composition-weighted elemental data following Ref. [17], giving $\lambda_{\text{Ti}} = 0.38$ and $\lambda_{\text{Ti-6Al-4V}} = 0.388$. As an independent check, the ABINIT electron-phonon calculation (Sec. II B) yields $\lambda = 0.548$ for elemental Ti directly from the Eliashberg spectral function, larger than the tabulated McMillan value. The product $\lambda \langle \omega^2 \rangle$, the quantity that actually enters Eq. (9), nevertheless agrees to within about 11% (216.4 meV² from ABINIT versus 243 meV² from the Debye-spectrum estimate), supporting the present parametrization. As the experimental Debye temperatures of Ti and Ti-6Al-4V are nearly identical (Table I) and the mean atomic mass changes by only about 4 %, $\lambda \langle \omega^2 \rangle$ is essentially material independent, so the computed difference in G is of electronic origin.

The lattice heat capacity $C_l(T_l)$ and lattice thermal conductivity $\kappa_l(T_l)$ were parametrized from experimental data. Functional forms are given in the Supplemental Material [41]. The experimental input data were taken from Refs. [64–67].

The simulation domain extended 1 μm into the bulk with grid spacing of 1 nm. Zero-flux boundary conditions were imposed at the surface and at the rear boundary. The coupled equations were integrated numerically with COMSOL Multiphysics version 6.4 [68].

The KKR formalism and the AAM are formally defined for crystalline solids. Lattice temperatures above about 1.3 T_m , the estimated threshold for ultrafast homogeneous melting under isochoric conditions [69], therefore extend the present treatment beyond its strict domain of validity. These data were retained as a first-order approximation, since the electronic DOS of close-packed metals changes only weakly upon melting [70].

III. RESULTS AND DISCUSSION

A. Equilibrium electronic transport in Ti

Figure 1(a) compares the calculated resistivity of hcp Ti with the experimental data of Bel'skaya *et al.* [71]. Both computational approaches, the KG calculation within SPR-KKR ($T_e = 0$ K, since electron-electron scattering $\ll$ electron-phonon scattering in equilibrium [13]) and the ABINIT electron-phonon calculation, reproduce the measured resistivity well at moderate temperatures, with values at 300 K of 54.3 $\mu\Omega\text{ cm}$ and 45.3 $\mu\Omega\text{ cm}$, respectively, compared with the experimental 47.5 $\mu\Omega\text{ cm}$, and with mutual agreement between the two methods up to about 700 K. Above this range the two methods diverge. The ABINIT result continues to rise over

the entire temperature range, as expected from the standard diffusive transport picture, which yields a linearly increasing scattering rate at high T . The experimental resistivity, in contrast, deviates from linearity above about 700 K and saturates close to the hcp–body-centered cubic (bcc) phase transition at about 1155 K. The sharp decrease of roughly 5% observed around this temperature is attributed to the structural transformation. The KG calculation reproduces the preceding resistivity saturation. The bcc phase above 1155 K was not included in either calculation, so the computed saturation arises entirely within the hcp CPA-AAM framework and is not associated with the structural transition.

The saturation of the KG resistivity is attributed to the progressive loss of quasiparticle coherence with increasing thermal disorder within the CPA-AAM framework. To quantify this, the quasiparticle coherence length ξ_i of each Fermi-surface sheet was extracted from the $\mathbf{k}$ -resolved occupation number $n(\mathbf{k})$, following the procedure of Robarts *et al.* [72]. The momentum distribution was obtained by integrating the Bloch spectral function [BSF, $A_B(\mathbf{k}, E)$] up to the Fermi energy,

$$n(\mathbf{k}) = \int_{-\infty}^{E_F} A_B(\mathbf{k}, E) dE. \quad (10)$$

For an ordered crystal, $n(\mathbf{k})$ exhibits sharp unit-step discontinuities at each Fermi-surface crossing, which are progressively smeared by thermal disorder. Each crossing was fitted with a hyperbolic tangent step function [72],

$$n(\mathbf{k}) = \sum_{i=1}^N \frac{c_i}{2} \left[1 + \tanh \left(\frac{4 \xi_i (\mathbf{k} - \mathbf{k}_{F,i})}{a} \right) \right] + C, \quad (11)$$

where $\mathbf{k}_{F,i}$ is the Fermi wave vector of the i th sheet, ξ_i the coherence length of that sheet along the given direction, c_i the step amplitude, and C a constant offset. The Fermi wave vectors were determined from a free fit at 0 K and held fixed at finite temperature, consistent with Luttinger's theorem [73]. The momentum distribution was sampled along seven special directions in the hcp BZ according to Ref. [74]. Fermi surface averaging of ξ_i over these directions gives the sheet-resolved electronic mean free path $\ell_{\text{mf},i}$. Individual paths are documented in the Supplemental Material [41].

Figure 1(b) shows the sheet-resolved mean free path $\ell_{\text{mf},i}/a$ for the four resolved Fermi surface sheets as a function of temperature. The mean free paths of all sheets decrease rapidly with temperature and saturate above about 1100 K at $\ell_{\text{mf},i}/a \approx 3$, corresponding to a mean free path of a few lattice constants, within a small factor of the Mott-Ioffe-Regel (MIR) limit $\ell_{\text{mf}} \approx a$. The finite values at 0 K, where no thermal disorder enters the AAM and the lattice is fixed, are an artifact of the finite imaginary energy $\text{Im} E = 1$ mRy used in the spectral-function evaluation. The saturation of ℓ_{mf} within the KKR-CPA-AAM formalism directly explains the resistivity saturation observed in Fig. 1(a). The inset shows the four tanh fits to $n(k)$ at 300 K for one of the seven evaluated paths. Analogous fits along the other directions yield qualitatively similar behavior.

To connect the electron mean free path to a resistivity estimate, the conductivity was evaluated in the relaxation-time

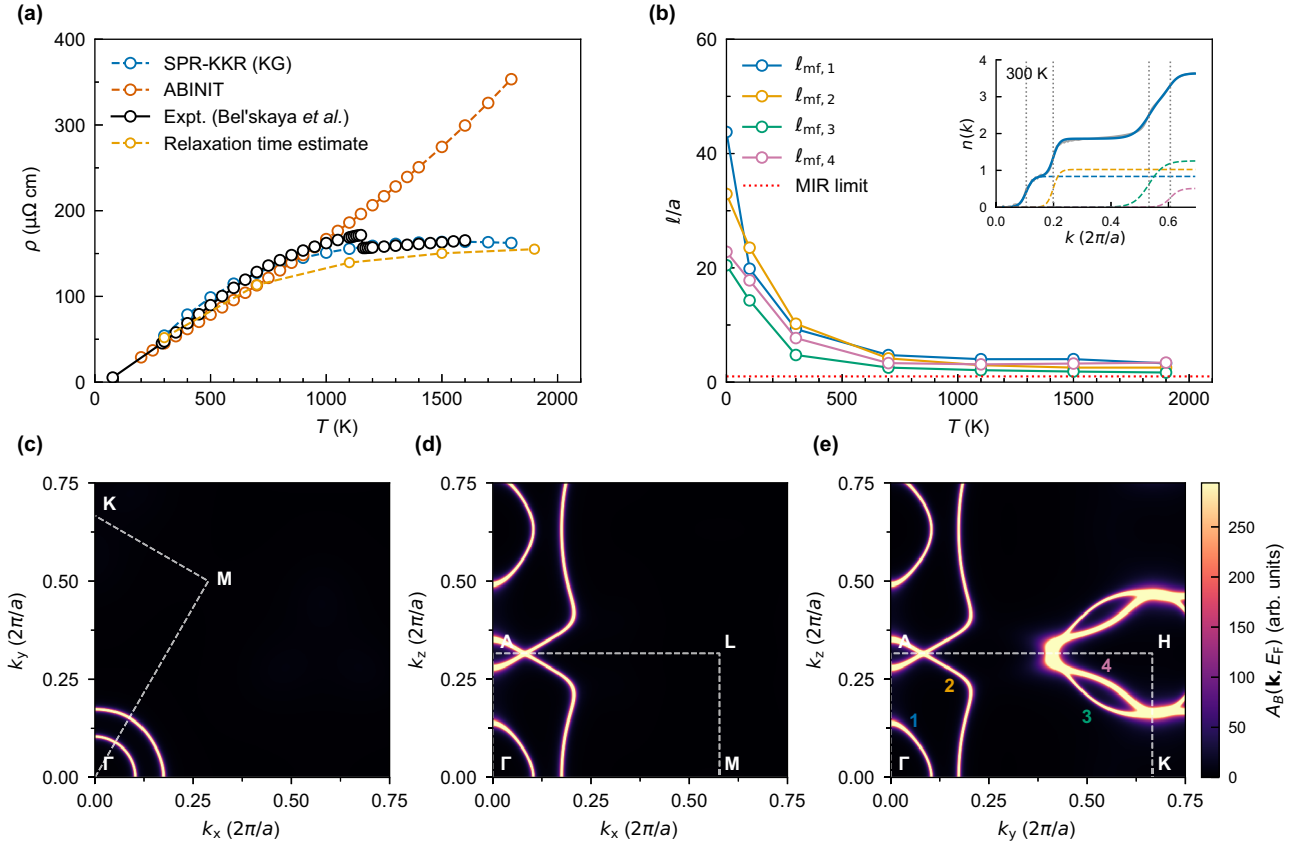


FIG. 1. Electronic transport and Fermi surface of hcp Ti from first-principles calculations. (a) Temperature-dependent electrical resistivity, showing the isotropic average from KKR-CPA KG calculations within SPR-KKR (blue), ABINIT results (orange), the relaxation time estimate from Eq. (12) (yellow), and experimental data from Bel'skaya *et al.* [71] (black). (b) Orientationally averaged, sheet-resolved mean free path $\ell_{mf,i}$ (in units of the lattice constant a) as a function of temperature, extracted from hyperbolic-tangent fits to the momentum distribution $n(k)$ along seven special directions [74]. Four Fermi-surface sheets are resolved: $\ell_{mf,1}$ (blue), $\ell_{mf,2}$ (yellow), $\ell_{mf,3}$ (green), and $\ell_{mf,4}$ (pink). The horizontal dotted line marks the MIR limit, $\ell_{mf} = a$. The inset shows the computed $n(k)$ at 300 K for one representative path together with the fit (blue) and the individual sheet contributions (dashed), with vertical dotted lines indicating the Fermi wave vectors. [(c)–(e)] Bloch spectral function $A_B(\mathbf{k}, E_F)$ at the Fermi energy, shown as plane cuts through the Γ point without thermal disorder (no AAM).

approximation [72],

$$\sigma_i = \frac{e^2}{12\pi^3\hbar} \ell_{mf,i} \mathcal{A}_i, \quad (12)$$

where $\mathcal{A}_i$ is the Fermi-surface area of sheet i . All sheets contribute in parallel, $\rho = (\sum_i \sigma_i)^{-1}$. The Fermi-surface is illustrated by the BSF at E_F without thermal disorder (no AAM), shown in Figs. 1(c)–1(e) as plane cuts through the Γ point. Four sheets are resolved: an inner, roughly ellipsoidal pocket around Γ (Sheet 1), an outer barrel-like hole extending along Γ -A (Sheet 2), and two zone-corner pockets near K and H (Sheets 3 and 4), all marked in Fig. 1(e). The overall shape agrees well with the Fermi surface reported by Souvatzis *et al.* [75]. The Fermi surface was located from the peaks of the Bloch spectral function on a mesh of 13 000 $\mathbf{k}$ points. The resulting iso-surfaces were triangulated and their areas integrated with the marching-cubes algorithm, with irreducible-wedge results scaled to the full zone using D_{6h} symmetry, giving $\mathcal{A}_1 = 0.168 (2\pi/a)^2$, $\mathcal{A}_2 = 0.840 (2\pi/a)^2$, $\mathcal{A}_3 = 1.368 (2\pi/a)^2$, and $\mathcal{A}_4 = 0.696 (2\pi/a)^2$. The full Fermi surface is shown in the Supplemental Material [41]. The resulting relaxation

time resistivity is included in Fig. 1(a). It agrees closely with the KG result, following the same temperature dependence, including the saturation. This confirms that the KG resistivity saturation is a direct consequence of the CPA-AAM treatment of thermal disorder, which limits the electronic mean free path at high lattice temperatures, consistent with the resistivity saturation found in first-principles transport studies of disordered transition-metal alloys [19].

B. Comparison of resistivity in Ti and Ti-6Al-4V

Figure 2 compares the electronic structure and equilibrium transport of hcp Ti and Ti-6Al-4V, including experimental resistivity data for both materials [71,76]. Figures 2(a) and 2(b) compare the BSF of hcp Ti and Ti-6Al-4V at 0 K. The band structure of Ti exhibits sharp, well-resolved bands throughout the BZ. In Ti-6Al-4V, chemical disorder among Ti, Al, and V introduces pronounced spectral broadening across all bands, reflecting the finite quasiparticle lifetime imposed by the disorder within the CPA. Despite this broadening, the overall band structure is preserved. The dominant d -band complex near E_F and the lower-lying sp -derived bands remain

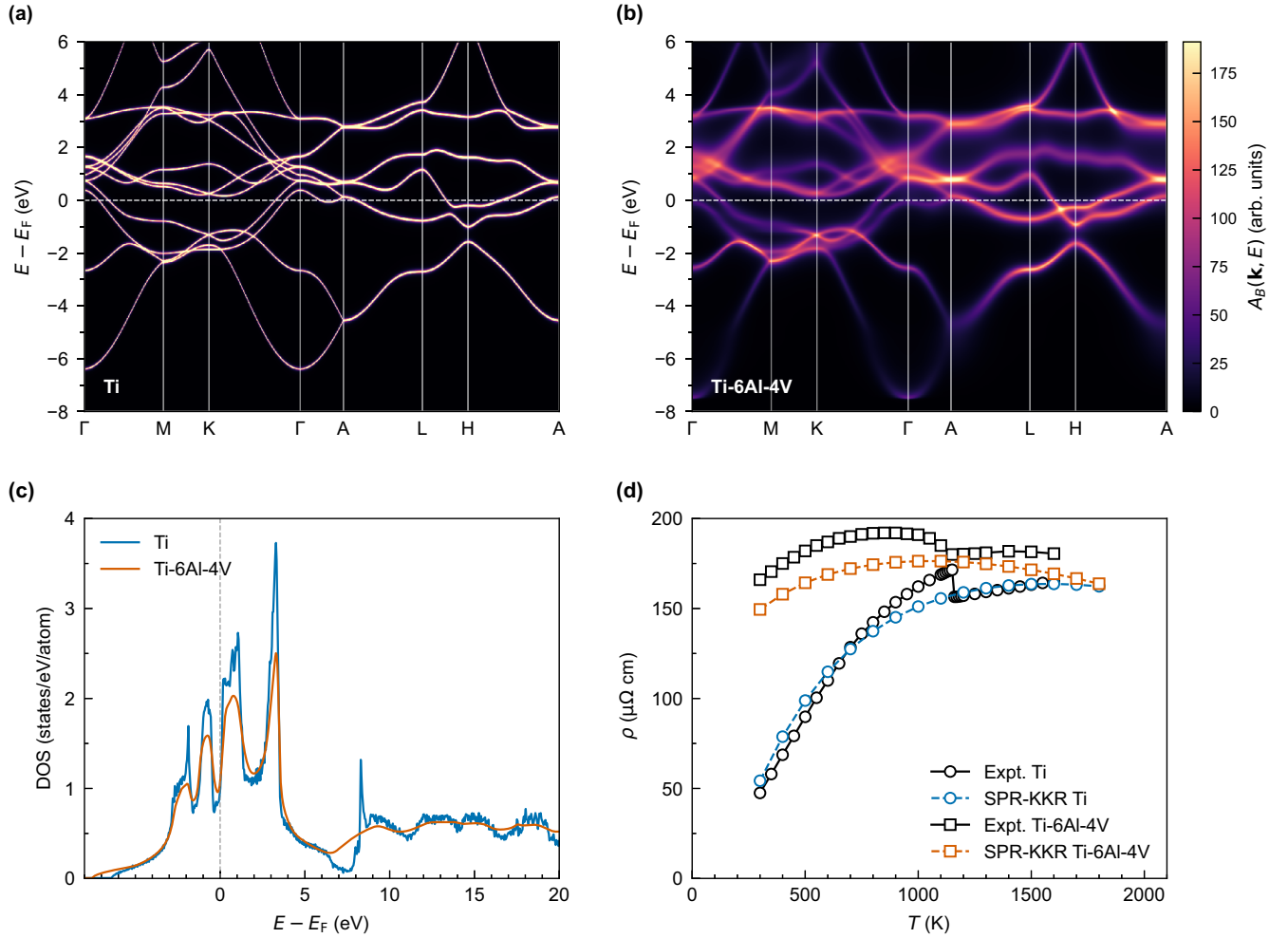


FIG. 2. Comparison of electronic structure and transport between hcp Ti and hcp Ti-6Al-4V. [(a) and (b)] BSF $A_B(\mathbf{k}, E)$ at 0 K along high-symmetry paths for Ti and Ti-6Al-4V, respectively. The dashed line marks E_F . (c) Total density of states per atom. The vertical dashed line indicates E_F . (d) Temperature-dependent electrical resistivity from KKR KG calculations (colored symbols) compared with experimental data (black symbols) for Ti [71] and Ti-6Al-4V [76].

recognizable, indicating that the alloy retains the essential electronic structure of titanium.

The primary electronic-structure effect of alloying is driven by aluminum. Although Al contributes one fewer valence electron than Ti, its sp states extend the occupied manifold about 1 eV further below E_F and, through $sp-d$ hybridization, reshape the d band near E_F , as shown by Woodgate *et al.* [77]. Vanadium, present at only 3.6 at.%, adds further disorder scattering but has a comparatively minor effect on the band structure.

These effects also appear in the density of states, shown in Fig. 2(c). The DOS of Ti-6Al-4V preserves the general shape of the Ti spectrum, but sharp features are systematically broadened, with peaks reduced in height and valleys partially filled.

Figure 2(d) shows the KG resistivity of both systems together with experimental data [71,76]. At low temperatures, the alloy resistivity is substantially higher than that of Ti, owing to a large residual resistivity of $120.3 \mu\Omega$ cm from chemical disorder [78], which acts as a temperature-independent elastic scattering channel. With increasing lattice

temperature, the difference between Ti and Ti-6Al-4V diminishes as thermal scattering shortens the electronic mean free path to a few lattice spacings, so that the additional chemical disorder contributes only marginally to the total resistivity. In Ti-6Al-4V the hcp-bcc transition is smeared out in experiment and the rapid resistivity drop seen in pure Ti is absent, yet the overall trend is nonetheless reproduced by the hcp calculation.

C. Electronic transport under electron-phonon nonequilibrium

USP laser irradiation transiently heats the electronic subsystem to several thousand Kelvin, far out of equilibrium with the lattice. The resulting transport and coupling properties are then determined by the finite- T_e electronic structure. The electronic thermal conductivity $\kappa_e(T_e)$ is not evaluated directly but is obtained from the generalized (Onsager) transport coefficients of Eq. (3), whose energy-resolved input is the KG conductivity $\sigma(E)$, computed at four lattice temperatures up to about $1.3 T_m$ for both materials.

Figure 3(a) shows $\sigma(E)$ for Ti at $T_l = 300$ K, evaluated across an energy window around E_F , extending beyond the

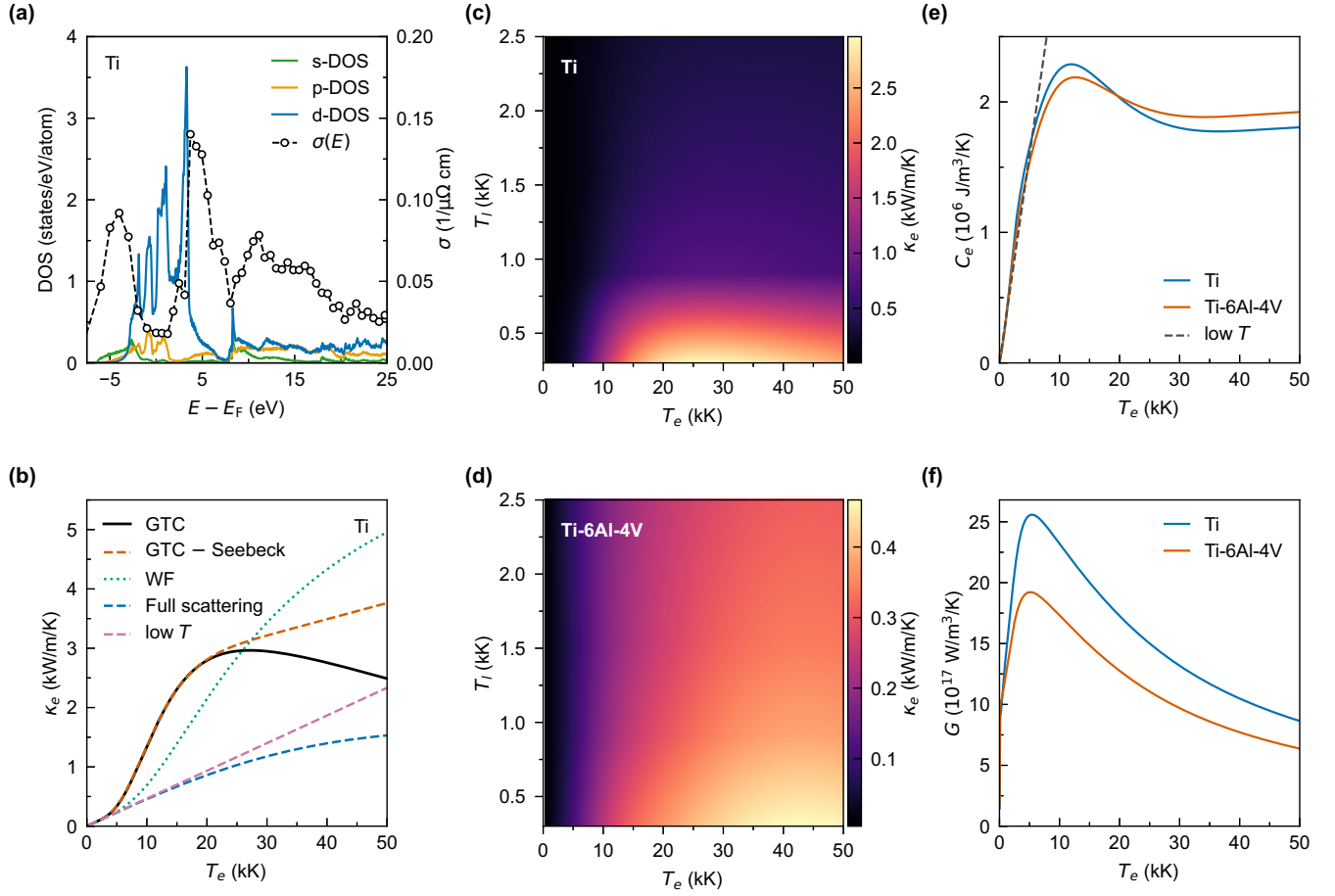


FIG. 3. Electronic properties of Ti and Ti-6Al-4V under electron-phonon nonequilibrium. (a) Orbital-resolved density of states (solid curves, left axis) and energy-resolved conductivity $\sigma(E)$ from KG calculations at $T_l = 300$ K (black circles, dashed line, right axis) for Ti; $\sigma(E)$ is suppressed where the d -DOS is large, as d states act as scattering centers. (b) Electronic thermal conductivity $\kappa_e(T_e)$ at $T_l = 300$ K for Ti: full GTC result from Eq. (4) (black solid) against four approximations (GTC without Seebeck correction, Wiedemann-Franz, the scattering model of Eq. (13), and the low- T model), which agree with GTC only below about 5 kK but diverge at higher electron temperatures. [(c) and (d)] Interpolated $\kappa_e(T_e, T_l)$ maps for Ti and Ti-6Al-4V, respectively, from GTC calculations at four lattice temperatures; the peak is a factor of 6.4 lower in the alloy. (e) Electronic heat capacity $C_e(T_e)$ from Eq. (8) for Ti and Ti-6Al-4V, nearly identical for both materials. (f) Electron-phonon coupling factor $G(T_e)$ from Eq. (9) for Ti and Ti-6Al-4V, where peak values differ by a factor of 1.3.

single value $\sigma(E_F)$ that enters the equilibrium resistivity, together with the band-resolved DOS. Near E_F , where the d -band contribution is largest, $\sigma(E)$ is suppressed, reflecting the role of the d states as a scattering channel for the mobile sp electrons rather than as a transport channel. Conversely, $\sigma(E)$ is large where sp character dominates. It peaks at 5 eV above E_F , where the d -band weight is minimal and remains large in the -7.5 to -2.5 eV range below E_F , before the onset of the d band. Above about 15 eV it falls off.

Figure 3(b) compares the resulting electronic thermal conductivity $\kappa_e(T_e)$ at $T_l = 300$ K, calculated from the full GTC expression in Eq. (4), alongside four approximations. The GTC result rises linearly at low T_e , with a room-temperature value of $13.5 \text{ Wm}^{-1} \text{ K}^{-1}$ for Ti, passes through a broad maximum near 27 kK, and decreases at higher T_e , a direct consequence of the Fermi window broadening into energy regions where $\sigma(E)$ decreases. Omitting the Seebeck correction [via $\kappa_e = L_{22}/(e^2 T_e)$ [52], orange dashed] overestimates κ_e by about 50% at 50 kK, because a temperature gradient

not only drives heat flow but also displaces charge carriers, and the resulting thermoelectric field opposes the thermal current. The Wiedemann-Franz law $\kappa_{\text{WF}} = \sigma(T_e) L_0 T_e$ (green dotted), with the electrical conductivity $\sigma(T_e)$ obtained from the Onsager coefficient L_{11} [52] and a constant Lorenz number L_0 , rises monotonically to nearly twice the GTC value at 50 kK, making it a poor estimate at high electronic temperature.

The electronic thermal conductivity can also be modeled within the Drude picture through the electron scattering rates [13], starting from the kinetic expression $\kappa_e = (1/3) C_e v^2 / \nu$ with the electronic heat capacity in its low-temperature Sommerfeld form $C_e = \gamma_e T_e$, the Fermi velocity $v = v_F$, and the total collision frequency split into electron-electron and electron-phonon contributions, $\nu = A_{ee} T_e^2 + B_{ep} T_l$. This yields

$$\kappa_e = \kappa_{e0} \frac{B_{ep} T_e}{A_{ee} T_e^2 + B_{ep} T_l}. \quad (13)$$

The electron-electron coefficient A_{ee} follows from the Quinn-Ferrell quasiparticle lifetime [79],

$$A_{ee} = \frac{(\pi k_B)^2}{2} K_{ee}, \quad K_{ee} = \frac{\sqrt{r_s}}{2 \cdot 3.98 \hbar E_F}, \quad (14)$$

where $r_s = (9\pi/4)^{1/3} \hbar / (a_0 \sqrt{2m_e E_F})$ is the Wigner-Seitz radius and a_0 the Bohr radius. The $(k_B T_e)^2$ scaling reflects the available Fermi-liquid phase space, while the $\sqrt{r_s}$ dependence enters through the random-phase-approximation screening of the Coulomb interaction. The numerical constant 3.98 is the Quinn-Ferrell screened-rate coefficient. For $E_F = 8.1$ eV ($r_s = 2.49$), $A_{ee} = 1.36 \times 10^6$ K⁻² s⁻¹. The electron-phonon coefficient $B_{ep} = \gamma_e v_F^2 / (3\kappa_{e0})$, with $v_F = \sqrt{2E_F/m_e}$ and $\gamma_e = 318$ J m⁻³ K⁻², is fixed by requiring Eq. (13) to recover the equilibrium conductivity at $T_e = T_l$. The equilibrium value κ_{e0} is taken as the Wiedemann-Franz value at 300 K (about 14 W m⁻¹ K⁻¹). This model (blue dashed) remains well below the GTC result, reaching only about half the GTC maximum within the plotted range (its turnover lies near 70 kK, beyond the plotted range), as it assumes free-electron transport and neglects the d -band structure.

In the electron-phonon-dominated low- T_e limit ($A_{ee} T_e^2 \ll B_{ep} T_l$), Eq. (13) reduces to $\kappa_e = \kappa_{e0} T_e / T_l$ (pink dashed), which rises linearly without bound. The electron-electron term $A_{ee} T_e^2$ in Eq. (13) progressively lowers κ_e relative to the linear low- T approximation, and a larger A_{ee} shifts the turnover to lower temperatures. Both scattering-rate models agree well with the GTC result below about 5 kK. Above that, a shortfall arises because they assume a constant DOS and an energy-independent free-electron conductivity, whereas $\sigma(E)$ rises markedly as $|E - E_F|$ increases [Fig. 3(a)]. As the Fermi window broadens with T_e , it samples these higher-conductivity states and raises κ_e above the free-electron estimate, an effect captured only by the GTC integration.

Figures 3(c) and 3(d) show the final $\kappa_e(T_e, T_l)$ maps used in the TTM, interpolated across the (T_e, T_l) plane from GTC calculations at four lattice temperatures. Ti reaches peak values of about 2970 W m⁻¹ K⁻¹ at low T_l and T_e near 27 kK, and the peak diminishes with increasing T_l as thermal disorder reduces $\sigma(E)$. Ti-6Al-4V peaks at only about 470 W m⁻¹ K⁻¹ at T_e near 43 kK, a factor of 6.4 lower, because chemical disorder suppresses $\sigma(E)$ at all energies. The T_l dependence is also weaker in the alloy, since thermal scattering adds only marginally to the already dominant chemical disorder, as already seen in the equilibrium transport [Fig. 2(d)].

The remaining electronic structure based parameters for the TTM are the heat capacity and the electron-phonon coupling factor. Figure 3(e) shows the electronic heat capacity $C_e(T_e)$ obtained from the DOS through Eq. (8). For both materials C_e rises with T_e and departs from the low-temperature Sommerfeld form $C_e = \gamma_e T_e$ as the Fermi window broadens into the structured d -band DOS, reaching a peak of 2.29 MJm⁻³ K⁻¹ for Ti and 2.19 MJm⁻³ K⁻¹ for Ti-6Al-4V near 12 kK, before decreasing as the window extends into regions of lower spectral weight. A Sommerfeld fit gives $\gamma_e = 318$ J m⁻³ K⁻² for Ti, with the alloy value moderately reduced, consistent with its broadened DOS near E_F . Figure 3(f) shows the electron-phonon coupling factor $G(T_e)$ evaluated through Eq. (9). For both materials G rises with T_e and reaches

a peak of approximately 25×10^{17} W K⁻¹ m⁻³ for Ti and 19×10^{17} W K⁻¹ m⁻³ for Ti-6Al-4V. The temperature dependence of both C_e and G for Ti agrees well with the data of Lin *et al.* [15], while the absolute magnitude of G is lower by a factor of about 1.5, reflecting the different $\lambda\langle\omega^2\rangle$ (a detailed comparison is given in the Supplemental Material [41]). While C_e is virtually identical for the two systems, the other electronic parameters differ significantly, with the peak values of G and κ_e varying by factors of 1.3 and 6.4, respectively.

D. Two-temperature model

The TTM response is evaluated at two thresholds, the melting threshold and the phase-explosion threshold. The melting threshold is taken as the onset of isochoric homogeneous melting, $T_{l,max} = 1.3 T_m$, which applies in the stress-confinement regime of ultrashort pulses [69]. Since the latent heat of fusion is incorporated as a Gaussian-smoothed transition in $C_l(T)$ centered at $1.3 T_m$ [80] (see Supplemental Material [41]), the simulated temperature must exceed this nominal criterion for the heat of fusion to be fully absorbed, so that the effective threshold is here defined as $1.4 T_m$. The phase-explosion threshold is taken as $T_{l,max} = 0.9 T_{crit}$, with $T_{crit} = 8980$ K the critical temperature of titanium [81].

For $\tau_p = 300$ fs, the threshold fluence is determined from the Ti calculation with 0.058 J/cm² for the melting threshold and 0.246 J/cm² for the phase-explosion threshold and then applied identically to Ti-6Al-4V and to a simplified Ti model in which the electronic thermal conductivity is replaced by the linear low- T form $\kappa_e = \kappa_{e0} T_e / T_l$. Figures 4(a) and 4(b) show the electron and lattice temperature evolution at the aforementioned thresholds. The Ti and Ti-6Al-4V first-principles parameter sets yield nearly indistinguishable lattice heating, with $T_{l,max} = 2722$ K and 2683 K respectively, a difference of only about 1.4%. The alloy nonetheless reaches a higher peak electron temperature ($T_{e,max} = 6127$ K versus 5585 K for Ti) and equilibrates more slowly (1.99 ps versus 1.72 ps), reflecting its lower electron-phonon coupling and conductivity. The low- T conductivity model yields $T_{l,max} = 2914$ K, overshooting the first-principles result by 7.1%. At the electron temperatures reached in this regime ($T_{e,max}$ near 5.6 kK), the linear model underestimates κ_e relative to the full GTC result, reducing electronic heat diffusion into the bulk and concentrating energy near the irradiated surface.

A similar pattern is observed in the phase-explosion regime. Ti and Ti-6Al-4V again yield nearly identical peak lattice temperatures (8091 K and 7980 K), while the alloy reaches higher $T_{e,max}$ (17.1 kK versus 15.5 kK) and equilibrates more slowly (2.27 ps versus 1.80 ps). The low- T conductivity model now overshoots $T_{l,max}$ by 19.1%, reaching 9638 K. The larger mismatch is consistent with Fig. 3(b). At $T_{e,max}$ near 16.8 kK the GTC thermal conductivity approaches its peak while the low- T approximation lies well below.

Across both regimes the conclusion is the same. The choice of functional form for κ_e introduces deviations in $T_{l,max}$ that are significantly larger than the difference between the first-principles Ti and Ti-6Al-4V parameter sets. The alloy-specific electronic structure modifies the electron dynamics but leaves the lattice thermal response nearly unchanged. This is consistent with experimental single-pulse ablation thresholds, which

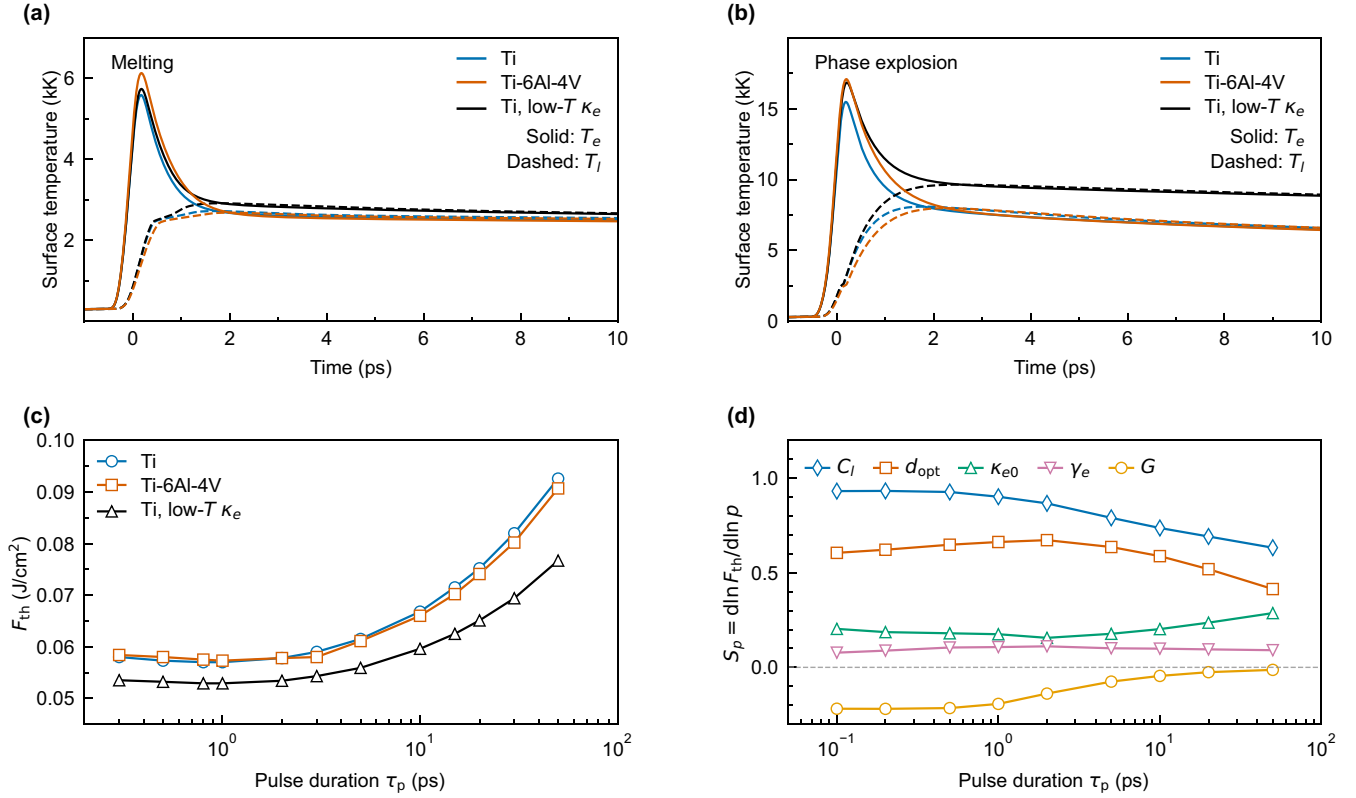


FIG. 4. Two-temperature dynamics and parameter sensitivity. [(a) and (b)] Calculated electron and lattice temperatures, T_e and T_l , for Ti, the simplified Ti model (with $\kappa_e = \kappa_{e0} T_e/T_l$), and Ti-6Al-4V after ultrashort-pulse excitation, at the melting threshold (a) and the phase-explosion threshold (b). (c) Melting-threshold fluence F_{th} as a function of pulse duration τ_p for the same three parameter sets. (d) Logarithmic sensitivity $S_p = d \ln F_{th} / d \ln p$ of the threshold fluence to the key model parameters as a function of pulse duration τ_p . Positive values indicate that increasing the parameter raises F_{th} , whereas negative values indicate a reduction.

for Ti ($0.28 \pm 0.02 \text{ J cm}^{-2}$ at 775 nm, 150 fs [82]) and Ti-6Al-4V ($0.272 \pm 0.021 \text{ J cm}^{-2}$ at 790 nm, 130 fs [83]) differ by only about 3%, well within the reported measurement uncertainties. Note that the peak lattice temperature serves only as a proxy for the ablation threshold. A quantitative comparison with measured thresholds would require an explicit ablation criterion, such as photomechanical spallation, which is beyond the scope of the present TTM.

Figure 4(c) shows the melting-threshold fluence F_{th} as a function of pulse duration τ_p from 300 fs to 50 ps for the three parameter sets. Ti and Ti-6Al-4V remain nearly indistinguishable up to 10 ps. In this range F_{th} is almost constant between 300 fs and 3 ps, passing through a shallow global minimum near 1 ps, and then rises with a square-root dependence, $F_{th} \propto \sqrt{\tau_p}$ [84]. Above 3 ps the Ti threshold increases relative to the alloy, reaching a difference of just above 2% at 50 ps.

Optimizing the pulse duration experimentally, however, requires the material response beyond the pure TTM. Efficient ablation demands operation within the stress-confinement regime [58,85], $\max(\tau_p, \tau_{ep}) < d_{eff}/c_l$, where $c_l = 4.4 \text{ km s}^{-1}$ [86] is the liquid sound velocity and $d_{eff} \approx d_{opt} = 20.4 \text{ nm}$ the effective energy-deposition depth, here the optical penetration depth. This gives a confinement time of 4.6 ps. The condition is met for both Ti and Ti-6Al-4V through the pulse duration rather than the electron-phonon equilibration time, which is estimated from Ref. [87] as $\tau_{ep} = \gamma_e T_e / G$. For the maximum electron temperature reached here, $T_e \approx 6 \text{ kK}$ at the 300 fs

melting threshold, and with G taken at its 300 K value, this yields $\tau_{ep} \approx 2 \text{ ps}$, in good agreement with the TTM dynamics in Fig. 4.

Within the stress-confinement regime, ablation proceeds through spallation, which is the most efficient removal mechanism and produces clean crater rims [88]. Pulse durations below 5 ps are therefore preferable. Beyond this range the process crosses over into the photothermal regime, accompanied by the additional heat dissipation apparent in the TTM [84,85,89].

Replacing the first-principles thermal conductivity with the low- T approximation lowers F_{th} by roughly 8% across all pulse durations below 2 ps, consistent with the 7% higher lattice temperature at equal fluence seen in Fig. 4(a) and by up to 17% at 50 ps. The deviation is thus itself pulse-duration dependent, indicating that the sensitivity of the threshold to the individual parameters varies with pulse duration.

Therefore, a logarithmic sensitivity analysis of the melting-threshold fluence F_{th} was performed on a linearized TTM with $C_e = \gamma_e T_e$, $\kappa_e = \kappa_{e0} T_e/T_l$, and constants C_l and G . Each parameter $p \in \{C_l, d_{opt}, \kappa_{e0}, \gamma_e, G\}$ is varied independently by $\pm \delta = \pm 10\%$ around the baseline p_0 . The logarithmic sensitivity $S_p \equiv d \ln F_{th} / d \ln p$ is approximated by the central difference $S_p = (\Delta F_+ - \Delta F_-) / (2\delta F_{th}(p_0))$, where $\Delta F_{\pm} = F_{th}(p_0(1 \pm \delta)) - F_{th}(p_0)$ is the threshold shift when parameter p is varied by $\pm \delta$ around its baseline value p_0 .

Figure 4(d) shows the resulting sensitivities as a function of pulse duration. G (yellow circles) and κ_{e0} (green triangles), which differ the most between the two materials in the present model, carry opposite sign. A reduction in G lowers the energy transfer rate to the lattice. A simultaneous reduction in κ_e confines the deposited energy closer to the surface, which in isolation would lower the threshold. Because both parameters are reduced in the alloy (see Fig. 3), the two effects largely cancel, explaining the near-identical lattice thermal response observed above.

At short pulse durations τ_p , G carries its largest electronic sensitivity, as the lattice heating rate is limited by electron-phonon energy transfer. With increasing pulse duration the two subsystems equilibrate during the pulse and $|S_G|$ approaches zero. This is consistent with G not being included in the threshold condition for long pulse durations via $F_{th} \propto \sqrt{\kappa_{e0} C_l \tau_p}$ [90]. Consequently, the sensitivity of κ_{e0} follows the opposite trend. It passes through a shallow minimum near $\tau_p = 2$ ps and rises to about 0.29 at 50 ps, as pulse-integrated thermal diffusion becomes the dominant heat-transport channel. The cancellation between S_G and $S_{\kappa_{e0}}$ is therefore most effective at short pulse durations and weakens in the picosecond regime, where κ_{e0} begins to dominate among the electronic parameters. The sensitivity of γ_e remains nearly flat at about 0.1 throughout, since the absorbed energy must be deposited into the electronic system regardless of pulse duration. The lattice heat capacity C_l and the optical penetration depth d_{opt} dominate the absolute sensitivity at all pulse durations.

The short-pulse limit corresponds to the analytical threshold derived by Corkum *et al.* [87] and Wellershoff *et al.* [91] for an idealized delta pulse shape ($\tau_p \rightarrow 0$) absorbed in an infinitesimal surface layer,

$$F_{th}^{Well} = \left(\frac{128}{\pi} \right)^{1/8} \left(\frac{\kappa_{e0}^2 C_l^5 T_m^3}{\gamma_e G^2} \right)^{1/4}, \quad (15)$$

which yields the exponents and thus the sensitivities of $(S_{C_l}, S_{d_{opt}}, S_{\kappa_{e0}}, S_{\gamma_e}, S_G)_{Well} = (5/4, 0, 1/2, -1/4, -1/2)$. The numerical sensitivities at $\tau_p = 0.2$ ps reproduce the ordering of the dominant exponents but are systematically reduced in magnitude, particularly for κ_{e0} and G .

This deviation can be traced to the assumption of instantaneous, pure surface absorption ($\tau_p \rightarrow 0, d_{opt} \rightarrow 0$) underlying Eq. (15), which removes d_{opt} from the threshold by construction. In the numerical TTM, d_{opt} sets the dominant deposition length scale for titanium, which transfers sensitivity away from the electronic diffusion parameters κ_{e0} and G toward d_{opt} , raising $S_{d_{opt}}$ to about 0.62 while reducing $|S_{\kappa_{e0}}|$ and $|S_G|$ relative to Eq. (15).

When $\tau_p \gg \tau_{ep}$, the two subsystems equilibrate during the pulse and the TTM reduces to one-temperature heat diffusion with $F_{th} \propto \sqrt{\kappa_{e0} C_l \tau_p}$ [90], resulting in $S_{C_l} \rightarrow 1/2$. The numerical sensitivities interpolate smoothly between these two analytical limits. Because $|S_G|$ vanishes while $S_{\kappa_{e0}}$ grows toward long pulses, the G - κ_{e0} compensation that renders Ti and Ti-6Al-4V nearly identical at femtosecond durations breaks down. Here the response becomes increasingly governed by the equilibrium thermal conductivity [$\kappa_e(T_e = T_l)$]. Averaging the equilibrium thermal conductivity up to the melting range yields a ratio of 1.19 for Ti/Ti-6Al-4V. With the long-pulse

sensitivity limit of 0.5, reached for pulse durations of several hundred ps to ns, Ti is then expected to exhibit a 9% higher ablation threshold than Ti-6Al-4V. The onset of this trend is already visible as the 2% difference at 50 ps from the TTM results above.

IV. CONCLUSION

Alloys are central to laser micromachining and surface-functionalization applications, yet predictive ultrashort-pulse laser simulations are frequently constrained by the absence of alloy-specific electronic material parameters. This limitation is particularly evident for Ti-6Al-4V, for which simulations have commonly relied on parametrizations derived from elemental Ti.

The temperature-dependent electrical resistivity, the electronic thermal conductivity, electronic heat capacity, and the electron-phonon coupling of hcp Ti and Ti-6Al-4V were computed, providing a comprehensive alloy-specific, fully temperature-dependent electronic parameter set for two-temperature modeling.

For Ti, the KG resistivity reproduces the experimentally observed high-temperature saturation, traced to the progressive loss of quasiparticle coherence within the CPA-AAM framework. The alloy retains the essential band topology of Ti but disorder introduces substantial spectral broadening and a large residual resistivity of $120.3 \mu\Omega \text{ cm}$ from chemical disorder. The electronic thermal conductivity κ_e , obtained from the full generalized (Onsager) transport coefficients, saturates and decreases at high T_e for both materials, peaking a factor of 6.4 lower in the alloy (about 470 versus $2970 \text{ W m}^{-1} \text{ K}^{-1}$), a behavior not captured by commonly used approximations.

In TTM simulations at the melting and phase-explosion thresholds, the first-principles Ti and Ti-6Al-4V parameter sets yield nearly identical peak lattice temperatures (within about 1.4%), despite a large difference in G , which peaks at 25 versus $19 \times 10^{17} \text{ W K}^{-1} \text{ m}^{-3}$ in Ti and Ti-6Al-4V respectively. A logarithmic sensitivity analysis dependent on pulse duration shows that the sensitivities of G and κ_e are of comparable magnitude but opposite sign, canceling each other out. Thus, the simulated melting-threshold fluences of the two materials differ by at most about 2% for pulse durations ranging from 300 fs to 50 ps, consistent with reported experimental single-pulse ablation thresholds, which agree to within about 3%.

Replacing the first-principles electronic thermal conductivity with the commonly used low temperature approximation, shifts $T_{l,max}$ by up to 19% for Ti. The functional form of the transport model therefore carries greater weight for predictive TTM accuracy in the ultrashort pulse regime than the distinction between Ti and Ti-6Al-4V.

The resulting dataset provides an alloy-specific first-principles basis for calculating transient electron and lattice temperatures in Ti-6Al-4V without substituting elemental-Ti transport properties. More broadly, our approach establishes a transferable framework for deriving electronic transport and thermophysical parameters of chemically disordered alloys under electron-phonon nonequilibrium at finite temperatures. Coupling such parameter sets to phase-transition, mechanical, hydrodynamic and molecular dynamic models should enable

increasingly quantitative predictions of ablation thresholds, material-removal efficiency, and processing quality in technologically relevant alloys.

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The authors declare no competing interests.

DATA AVAILABILITY

The numerical data and analysis scripts that support the findings of this study are openly available on Zenodo [92].

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