

An *ab Initio* Answer to Long-Debated Questions about Superconducting Nb₃Sn

Alessio Cucciari^{✉*} and Lilia Boeri^{✉†}

Dipartimento di Fisica, *Sapienza Università di Roma*, 00185 Rome, Italy



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Nb₃Sn is the workhorse superconductor for high-field applications; however, several fundamental aspects remain open 70 years after its discovery. Using anharmonic *ab initio* Migdal-Eliashberg theory, we resolve three key questions: (1) the cubic-to-tetragonal martensitic transition is weakly first order; (2) the superconducting gap is strongly anisotropic but continuous over the Fermi surface; and (3) the drop of H_{c2} across the transition arises from both reduced electron-phonon coupling and a redistribution of Fermi velocities. The orbital origin of the gap anisotropy suggests targeted doping strategies: Sn-site substitution can increase both T_c and H_{c2} , while Nb-site substitution raises H_{c2} at the cost of lowering T_c .

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I. INTRODUCTION

Whether or not the global race toward room-temperature superconductivity succeeds, many technologies will still rely on materials that operate under strong magnetic fields, rather than merely at high temperatures. These include magnetic resonance imaging, particle accelerators, and fusion reactors, which require superconductors with high upper critical fields H_{c2} , high critical current densities J_c , and scalable manufacturing.

High- T_c cuprates, such as rare-earth barium copper oxides, offer impressive performance, with H_{c2} exceeding 100 T [1], but strong anisotropy and fabrication costs have limited their widespread use. For this reason, low- T_c conventional superconductors such as Nb-Ti and Nb₃Sn remain the most practical choices, even decades after their discovery. Among them, Nb-Ti is more widely used but already operates near its intrinsic limits [2]. Meanwhile, Nb₃Sn is the leading candidate for next-generation magnets thanks to its higher T_c (18.3 K) and H_{c2} (up to 29 T) [3], and still offers potential for further optimization.

Nb₃Sn belongs to the A15 family of superconductors [4], a class of intermetallic compounds with general formula A_3B and preferred cubic symmetry (space group $Pm\bar{3}n$). These compounds feature a body-centered sublattice of B atoms (e.g., Sn) and three orthogonal chains of A atoms (e.g., Nb) along the cubic axes, as illustrated

in Fig. 1. Many A15 superconductors undergo a martensitic transformation [5]: upon cooling below a temperature $T_m > T_c$, nearly stoichiometric samples undergo a diffusionless structural transition to a tetragonal phase (space group $P4_2/mmc$) [6]. This transformation is driven by a zone-center optical phonon mode of symmetry Γ_{12}^+ , which induces a dimerization δ of the chains and couples linearly to a tetragonal strain $\varepsilon = c/a - 1$ [7]. As shown in Fig. 1, the Nb atoms shift alternately along the chain directions (red arrows), and the lattice distorts along one axis. The transition occurs at $T_m \approx 43$ K in Nb₃Sn, with measured $\varepsilon = -0.006$ and $\delta = -0.003$ [6,8]. In tetragonal samples compared with cubic samples, T_c is reduced, but, more importantly, H_{c2} drops from its optimal value of 29 T to about 21 T [2,9], suppressing practical performance.

For this reason, optimization of Nb₃Sn has relied on empirical strategies to prevent the martensitic transition. For instance, the introduction of impurities (such as Ti, Ta, or Hf) in small concentrations is known to stabilize the cubic structure and also increase H_{c2} , even if it slightly reduces T_c [10–13]. Theory-guided optimization, which could offer important hints on innovative design strategies [14], has so far been extremely limited. In contrast to for novel superconductors such as hydrides or borides, *ab initio* Migdal-Eliashberg (ME) theory fails for many technological superconductors. For example, in both Nb-Ti and Nb₃Sn, the underlying assumptions of *ab initio* ME theory—dynamically stable structure, perfectly stoichiometric crystals—break down [15–17]. Some studies circumvented this problem by artificially stabilizing the structure through increased electronic smearing [18–24], but this is physically unjustified. A proper treatment requires going beyond the harmonic approximation and including anharmonic effects. Such calculations were computationally unfeasible until recently, but thanks to the combination

*Contact author: alessio.cucciari@uniroma1.it

†Contact author: lilia.boeri@uniroma1.it

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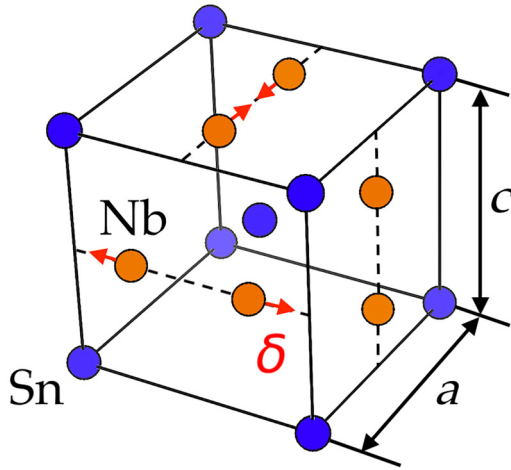


FIG. 1. Crystal structure of A15 Nb_3Sn . Nb (orange) and Sn (blue) atoms occupy Wyckoff positions $6c$ and $2a$, respectively.

of the stochastic self-consistent harmonic approximation (SSCHA) with machine-learning interatomic potentials (MLIPs) [25–27], it is now possible to include these effects microscopically, as we have demonstrated for Nb-Ti [15].

In this work, we perform state-of-the-art *ab initio* calculations to provide a fully microscopic description of the superconducting state of Nb_3Sn . To do this, we address several open questions that are critical for guiding material optimization. In particular, we address three unresolved issues. First, the thermodynamic nature of the martensitic transition: Anderson and Blount [28] showed that a cubic-to-tetragonal transformation should be first order in the absence of any change in internal symmetry other than mere strain. However, in V_3Si the transition is second order [29,30], while for Nb_3Sn results are unclear [30–33]. Second, the anisotropy of the superconducting gap: Early specific heat and point-contact spectroscopy studies suggested a two-gap scenario [34,35], while more recent measurements hint at a single gap [32,36]. A detailed understanding of the gap anisotropy is crucial for wire design, as it governs vortex formation and pinning and directly impacts both H_{c2} and J_c . Third, the role of the phase transition in suppressing H_{c2} : recent reports challenge the established idea that H_{c2} drops due to the martensitic transition to the tetragonal phase [37], leaving the microscopic origin of this suppression unclear.

This paper is organized as follows. In Sec. II, we discuss the nature of the martensitic transition, describing the profile of the Born-Oppenheimer surface and its anharmonic generalization. In Sec. III, we examine the electronic structures of the cubic and tetragonal phases. In Sec. IV, we report the anharmonic phonon spectra computed via the SSCHA-MLIP method, while in Sec. V, we discuss the superconducting properties obtained from the solution of the anisotropic Migdal-Eliashberg equations and analyze

possible optimization strategies. A summary of our key findings is given in Sec. VI. Technical details of the calculations are provided in Sec. VII.

II. MARTENSITIC TRANSITION

To investigate the origin of the martensitic transition in Nb_3Sn , we computed its Born-Oppenheimer potential energy surface at fixed volume, as the real transition involves only volume changes that can be safely ignored. We used density functional theory (DFT) with the PBEsol exchange-correlation functional [38], which is known to be more accurate than the standard Perdew-Burke-Ernzerhof functional. Further computational details are given in Sec. VII. Results are shown in Fig. 2(a), where the ground state energy of the system is plotted as a function of two structural order parameters: the tetragonal strain $\varepsilon = c/a - 1$ (horizontal axis) and the Nb-chain dimerization δ (vertical axis), which corresponds to the eigenvector of the

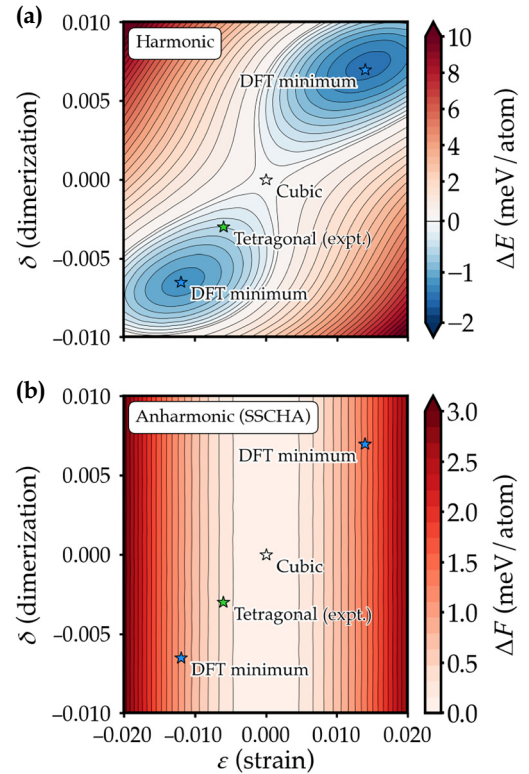


FIG. 2. (a) Contour plot of the fixed-volume Born-Oppenheimer potential energy surface $\Delta E(\varepsilon, \delta)$ computed with DFT. The energy is given relative to the cubic configuration ($\varepsilon = 0, \delta = 0$), which corresponds to a saddle point (white star). Two locally stable minima (blue stars) are located at $(-0.012, -0.006)$ and $(0.014, 0.007)$, while a green star indicates the experimentally observed distortion. (b) Same as (a), but including zero-point energy corrections through the SSCHA. ΔF denotes the resulting anharmonic free energy difference relative to the cubic configuration, which serves again as a reference.

TABLE I. Crystallographic data for cubic and tetragonal (experimental) Nb₃Sn structures. Lattice parameters for the cubic phase are obtained from SSCHA relaxation at zero pressure. Lattice parameters for the tetragonal phase were chosen to maintain the same unit-cell volume.

Phase	Space group	Lattice parameters (Å)	Atomic site (Wyckoff position)	<i>x</i>	<i>y</i>	<i>z</i>
Cubic	$Pm\bar{3}n$ (223)	$a = b = c = 5.264$	Sn (2 <i>a</i>)	0.0000	0.0000	0.0000
			Nb (6 <i>c</i>)	0.0000	0.5000	0.2500
Tetragonal	$P4_2/mmc$ (131)	$a = b = 5.276, c = 5.241$	Nb (2 <i>c</i>)	0.0000	0.5000	0.0000
			Nb (2 <i>f</i>)	0.5000	0.5000	0.2500
			Sn (4 <i>j</i>)	0.2468	0.0000	0.0000

Γ_{12}^+ optical phonon, as defined in Fig. 1. The color scale indicates the total energy per atom relative to the cubic configuration ($\varepsilon = 0, \delta = 0$), with red and blue indicating higher and lower energies, respectively, and thus representing the depth of the energy landscape. Figure 2(a) reveals a double-well profile, with two slightly asymmetric minima (blue stars) separated by a shallow energy barrier of less than 2 meV/atom. A saddle point (white star) occurs at (0, 0), i.e., the cubic phase. This result is in excellent agreement with earlier calculations and confirms that the cubic phase of Nb₃Sn is dynamically unstable at the harmonic level [16,17]: the unstable Γ_{12}^+ phonon induces a dimerization δ of the Nb chains that makes the system collapse into one of the tetragonal minima. This dynamical instability can be artificially suppressed by increasing the electronic smearing, as shown in Fig. S1 in Supplemental Material [39].

On the basis of Fig. 2(a), DFT predicts the martensitic transition to be a second-order Peierls-like transition, as proposed by early semiphenomenological models [7]. DFT in the harmonic approximation also overestimates the equilibrium values of ε and δ by approximately a factor of 2 compared with experiments. However, the energy difference between the theoretical and experimental minima is small, about 0.5 meV/atom, i.e., within the typical accuracy of DFT calculations. We show in Sec. V that the tetragonal phase is also dynamically unstable within the harmonic approximation, although its instability is associated with different phonon eigenvectors.

Since phonons are unstable at the harmonic level, but crystals are experimentally stable, we used the SSCHA to assess whether anharmonicity would restore the correct energy landscape. At $T = 0$ K, anharmonic effects contribute through quantum zero-point fluctuations. The resulting landscape differs qualitatively from the harmonic one—see Fig. 2(b): the cubic configuration becomes the global minimum of a broad and shallow well, of depth approximately 3 meV/atom. When tetragonal structures are relaxed within the SSCHA, they always relax back to the cubic structure. Thus, within the accuracy of the SSCHA calculations, the cubic structure remains the stabler at all temperatures, even below the experimental transition temperature T_m .

At first sight, this result seems to contradict experiments, which report a clear structural transition to a tetragonal phase below T_m . However, experimentally, the transition appears only in nearly perfectly stoichiometric samples, and even slight deviations from stoichiometry are sufficient to suppress the transition, stabilizing the cubic phase below T_m [2,40]. Moreover, within the SSCHA, all tetragonal configurations ($\varepsilon \neq 0$) are associated with anisotropic internal stress. In the experimental configuration ($\varepsilon_{\text{expt}} = -0.006, \delta_{\text{expt}} = -0.003$), the difference between the axial and in-plane stress components is about 0.3 GPa, in good agreement with the residual stress that is measured in Nb₃Sn wires produced by the bronze method [41]. This suggests that residual stress—arising from compositional inhomogeneity, volume contraction during Nb₃Sn formation, and thermal-expansion mismatch with the surrounding matrix—can stabilize the tetragonal phase in practical samples, sustaining the distortion despite the associated energetic cost. Thus, synthesis methods that reduce residual internal stress, such as slower cooling rates, incorporation of additional stress-relief annealing steps following Nb₃Sn formation, or alternative synthesis methods such as epitaxial growth (which enables direct control of strain through substrate selection), may suppress the martensitic transition and stabilize the cubic phase. Recent efforts to use epitaxial growth for radio-frequency cavity applications have shown promise [42], although achieving high Sn content remains challenging due to the limited diffusion of Sn in the absence of a Cu matrix.

Since within the SSCHA we could not find a minimum for the tetragonal structure [43], in the rest of this work we adopt the experimental tetragonal structure as a reference for comparison with the cubic phase. Hereafter, we refer to the latter as “the cubic phase” and to the former as “the tetragonal phase.” Crystallographic data are reported in Table I.

III. ELECTRONIC STRUCTURE

We now discuss in detail the electronic structure of the two phases. The band structures of cubic and tetragonal Nb₃Sn are illustrated in Fig. 3. In Fig. 3(a), we report the band structure of the cubic phase. The thickness of

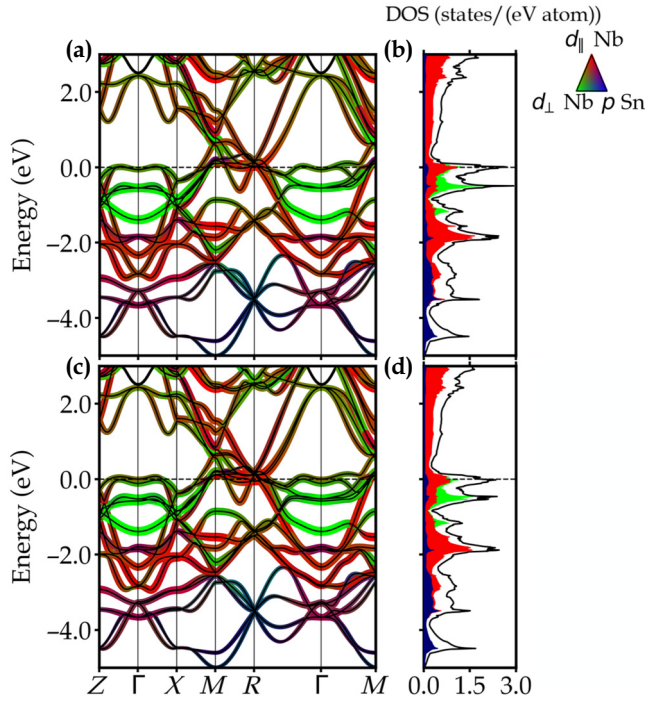


FIG. 3. (a),(c) Electronic band structure of cubic and tetragonal Nb_3Sn . The thickness of each band reflects the weight of the projected orbitals: Nb $d_{\parallel}$ (red), Nb $d_{\perp}$ (green), and Sn p (blue). $d_{\parallel}$ denotes Nb d orbitals oriented along the direction of the corresponding Nb—Nb chains, while $d_{\perp}$ indicates d orbitals transverse to the chains. (b),(d) Orbital-projected DOS. The total DOS is shown in black. The Fermi level is set to zero energy (dashed line).

each band indicates the orbital character of the electronic states. We project the Bloch states onto three main orbital components: Nb $d_{\parallel}$ (red), Nb $d_{\perp}$ (green), and Sn p (blue) orbitals. Here $d_{\parallel}$ is the subset of Nb d orbitals oriented longitudinally along the corresponding Nb—Nb chain of the A15 structure, and $d_{\perp}$ represents transverse d orbitals, i.e., orthogonal to the chain direction.

Valence bands extend about 5 eV below the Fermi level. In the energy range from -5.0 to -3.0 eV, the dominant character is Sn p , with a noticeable contribution from Nb s states. Nb d orbitals contribute significantly across the entire valence region. Close to the Fermi level, the spectral weight is almost entirely due to Nb d orbitals, as indicated by the orbital-projected density of states (DOS) reported in Fig. 3(b). The total DOS $N(\epsilon)$ displays several sharp features, including a prominent peak at the Fermi level ϵ_F , where $N(\epsilon_F) = 2.4$ states/(eV atom). This peak arises from flat, nearly dispersionless bands that cross ϵ_F in all directions around the Γ point and along the M - R directions. These flat bands display a mixture of longitudinal ($d_{\parallel}$) and transverse ($d_{\perp}$) Nb orbital character: near the R point, $d_{\parallel}$ states dominate, while near the Γ , point, the $d_{\perp}$ component becomes dominant, accounting for up to 75%

of the total orbital weight. Additionally, a flat band along the M - R path is characterized primarily by Sn p orbitals. A fourfold-degenerate manifold at the R point is located only a few millielectronvolts above the Fermi level and generates several highly dispersive conduction bands. These bands, which cross ϵ_F with high Fermi velocity, are mainly of $d_{\parallel}$ character. The resulting Fermi surface consists of six sheets (see Figs. S3–S5 in Supplemental Material [39]): four tubular sheets along the Brillouin zone edges, reflecting the chainlike $d_{\parallel}$ states from the M - R region, and nearly spherical electron pockets around the Γ point, dominated by $d_{\perp}$ orbitals. A more detailed discussion of this orbital decomposition of the Fermi surface is provided in Sec. V.

In Figs. 3(c) and 3(d), we report for comparison the band structure and DOS of the tetragonal phase of Nb_3Sn . As noted in earlier studies [16,19], the tetragonal strain $\epsilon = c/a - 1$ does not cause significant changes in the electronic structure. However, the dimerization δ has a much stronger effect, splitting several flat bands near the Fermi level, particularly at the Γ and R points. These bands, nearly dispersionless in the cubic phase, lose their degeneracy and shift upwards and downwards in energy in the low-symmetry phase, reducing the DOS at the Fermi level by 16%. As a consequence, one of the bands becomes fully occupied. This makes the Γ_{12}^+ phonon potential anharmonic, as the energy gain from band splitting depends nonlinearly on δ . The magnitude of the anharmonic correction depends on $N(\epsilon_F)$ [44]. This explains why increasing the electronic smearing stabilizes the phase: smearing smooths out sharp features in the DOS, artificially reducing $N(\epsilon_F)$ and suppressing the instability.

IV. VIBRATIONAL PROPERTIES

We now discuss the vibrational properties of the two phases of Nb_3Sn . In Figs. 4(a) and 4(d), we compare the phonon dispersions obtained from harmonic density functional perturbation theory (DFPT; dashed lines) and the SSCHA (solid lines) at $T = 0$ K. At the harmonic level, both cubic and tetragonal Nb_3Sn are dynamically unstable: as expected from the ϵ vs δ plots shown in Fig. 2(a), the zone-center Γ_{12}^+ phonon mode (highlighted with red circles) has imaginary frequencies in the cubic phase but real frequencies in the tetragonal phase, where other instabilities emerge at the X and Z points. Once anharmonic effects are included with the SSCHA, all imaginary frequencies disappear, and both phases become dynamically stable. The Γ_{12}^+ mode, in particular, undergoes a strong renormalization (red stars). Taken together, these results support the scenario evidenced in Fig. 2(b): the martensitic transition in Nb_3Sn is not a Peierls-like second-order transition, driven by a soft mode, but is rather a weakly first-order transition between two nearly degenerate minima, both stabilized by anharmonic effects. Which phase prevails depends on internal residual stress or on deviations

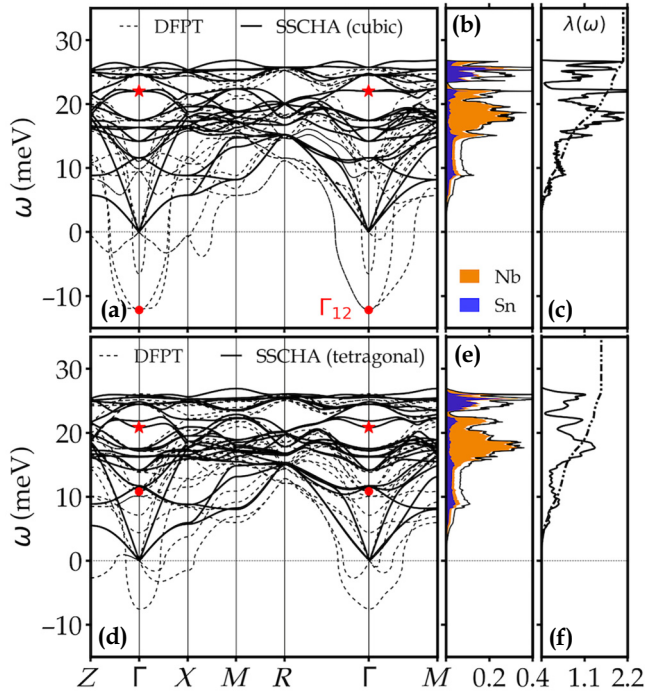


FIG. 4. (a),(d) Phonon dispersions computed within harmonic DFPT (dashed black lines) compared with fully anharmonic SSCHA calculations at $T = 0$ K (solid black lines) for the cubic phase and the tetragonal phase of Nb_3Sn , respectively. Negative frequencies represent imaginary phonon modes. Red circles denote the calculated DFPT frequency of the Γ_{12}^+ mode, which drives the transition. Red stars denote its renormalization due to anharmonic effects. (b),(e) Atom-projected and total phonon density of states in the unit of states/meV. Nb and Sn projections are represented in orange and blue, respectively. (c),(f) Isotropic Eliashberg spectral functions $\alpha^2F(\omega)$, along with the electron-phonon coupling $\lambda(\omega)$ (dotted-dashed black line).

from stoichiometry that can lower the cubic minimum compared with the tetragonal minimum.

The atom-projected phonon densities of states computed with SSCHA are shown in Figs. 4(b) and 4(e). The vibrational spectrum extends up to approximately 27 meV and can be divided into three regions. The low-frequency part (0–15 meV), associated with acoustic modes, is nearly identical in both phases and shows equal contributions from Nb and Sn atoms. In the mid-frequency range (15–21 meV), phonon modes related to Nb-chain vibrations, such as the Γ_{12}^+ phonon, dominate the spectrum. At higher frequencies, both Nb and Sn atoms contribute.

To validate our SSCHA calculations, we compare the anharmonic phonon dispersions computed with the SSCHA at $T = 0$ K and $T = 300$ K for the cubic phase with experimental inelastic neutron scattering data reported by Axe and Shirane [45] and Pintschovius *et al.* [46,47]—see Fig. 5(a). The samples analyzed in these studies undergo the martensitic transition and therefore become tetragonal below the transition temperature T_m . Although

the low-temperature data (5 K) are formally obtained in the tetragonal phase, they are reported only for the longitudinal acoustic branch, which remains nearly identical in the cubic and tetragonal structures, thereby justifying the comparison. Our calculations show excellent agreement with both datasets, reproducing not only the energy scale but also the curvature of all major phonon branches. In particular, our calculations accurately reproduce the temperature renormalization of the Γ_{12}^+ mode, reinforcing the reliability of the SSCHA approach. Minor deviations from the 46 K data of Axe and Shirane [45] (orange circles) are visible along the Γ - M path, where an anomalous softening of the longitudinal acoustic branch is experimentally observed [9]. This softening, related to the elastic constant $C_{11} - C_{12}$, is a well-known precursor of the martensitic transition, which occurs just above the transition temperature T_m and is restored below it, whether or not the transition occurs. Since our calculations are performed at $T = 0$ K, they are not expected to reproduce this anomaly, and indeed no such softening is observed, which is consistent with the rehardening of the elastic constant at low temperature [9]. We also note that our calculations do not reproduce the softening of the longitudinal acoustic branch along the Γ - R direction reported by Pintschovius *et al.* [47] (blue stars) at low temperature. This discrepancy is the only notable deviation from the experimental data. For reference, we report in Fig. S2 in Supplemental Material [39] the DFPT phonon dispersions of the cubic phase computed with a larger electronic smearing. While smearing artificially stabilizes the phonons, the resulting spectra deviate significantly from the experimental data, confirming that only a proper anharmonic treatment can explain the experimental data.

V. SUPERCONDUCTING PROPERTIES

A. Critical temperature

The isotropic Eliashberg spectral functions $\alpha^2F(\omega)$ of cubic and tetragonal Nb_3Sn are shown in Figs. 4(c) and 4(f) and are compared with experimental data from tunneling spectroscopy in Fig. 5(b) [48–53]. The positions of the dominant peaks are in excellent agreement with most literature reports, indicating that our calculations correctly capture the key features of the phonon spectrum. In both cubic and tetragonal Nb_3Sn , the frequency-dependent electron-phonon coupling $\lambda(\omega)$ increases linearly with phonon frequency, suggesting an even contribution from all phonon branches. The corresponding integrated electron-phonon coupling constants λ and logarithmic average phonon frequencies $\omega_{\log}$ are reported in Table II. Our calculated $\lambda = 2.08$ for the cubic phase is slightly larger than the experimental average $\lambda^{\text{expt}} = 1.83$ [54]. However, determination of λ in Nb_3Sn is notoriously challenging, both experimentally and computationally [26,50–52], due to the strong energy dependence of

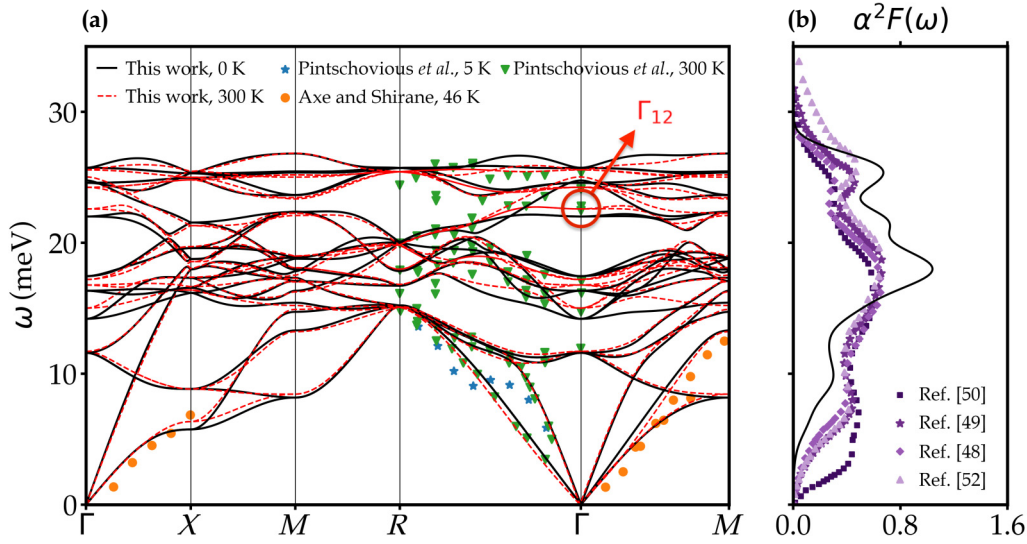


FIG. 5. (a) SSCHA phonon dispersions of cubic Nb₃Sn at $T = 0$ K and $T = 300$ K. The results show excellent agreement with inelastic neutron scattering data (colored markers) from Pintschovious *et al.* [46,47] and Axe and Shirane [45]. The temperature-dependent renormalization of the Γ_{12}^+ mode is accurately reproduced, providing a strong validation of our results. (b) Calculated Eliashberg spectral function $\alpha^2 F(\omega)$ compared with experimental data (purple markers) extracted from tunneling spectroscopy in Refs. [48–50,52]. The theoretical curve has been broadened to facilitate comparison with experimental results, which show a significant spread of shapes.

the electronic DOS near a van Hove singularity. Indeed, the van Hove singularity makes all calculated quantities extremely noisy [26]: to reduce this effect, we solved the anisotropic Migdal-Eliashberg equations by means of a full-bandwidth approach, as recently implemented in the EPW code [55]. Results are summarized in Table II, where they are compared with experimental data, if available. The Coulomb interaction is treated within the Morel-Anderson pseudopotential μ^* framework [56], with the use of μ^* values for the cubic phase derived from first-principles random-phase approximation and Kukkonen-Overhauser calculations by Pellegrini *et al.* [57]. Values for the tetragonal phase were obtained by rescaling of the cubic μ^* by

the DOS at the Fermi level—see Table S2 in Supplemental Material [39,53].

The superconducting gap $\Delta_{\mathbf{k}}$ of the two phases, shown in Fig. 6(a), displays a broad but continuous anisotropic distribution over the Fermi surface. In the cubic phase, the largest gap values (≈ 6.3 meV) are found near the corners of the Brillouin zone. Here, the Fermi velocity $v_F(\mathbf{k})$ is low and electronic states are dominated by longitudinal $d_{||}$ orbitals of the Nb chains—see Figs. S3–S5 in Supplemental Material [39]. In contrast, the smallest gap values (≈ 3.1 meV) appear on the electron pockets near the Γ point, where the Fermi velocity is low but electron-phonon coupling is weaker. As discussed in Sec. III, these

TABLE II. Calculated superconducting properties of cubic and tetragonal Nb₃Sn. $N(\epsilon_F)$ is the electronic DOS at the Fermi level; λ is the electron-phonon coupling constant; $\omega_{\log}$ is the logarithmically averaged phonon frequency; $\langle v_F \rangle$ is the average Fermi velocity over the Fermi surface; $\langle \Delta \rangle$ is the average superconducting gap; T_c and T_c^{expt} are the theoretical and experimental critical temperatures, respectively; $2\Delta/k_B T_c$ is the BCS ratio; $\langle \xi_0 \rangle$ is the average Pippard coherence length; $\xi^c(0)$ is the Ginzburg-Landau coherence length calculated at $T = 0$ K in the clean limit; ℓ^{expt} is the experimental electronic mean free path; $\xi^{\text{expt}}(0)$ is the experimental Ginzburg-Landau coherence length; $H_{c2}^c(0)$ is the upper critical field at $T = 0$ K, calculated in the clean limit and with Pauli limiting ignored; $H_{c2}^{\text{expt}}(0)$ is the experimental upper critical field measured in nearly stoichiometric samples. Experimental data are taken from Refs. [54,60].

Phase	$N(\epsilon_F)$ [states/(eV atom)]	λ	$\omega_{\log}$ (meV)	$\langle v_F^* \rangle$ (10^7 cm/s)	$\langle \Delta \rangle$ (meV)	T_c (K)	T_c^{expt} (K)	$2\Delta/k_B T_c$	$\langle \xi_0 \rangle$ (nm)	$\xi^c(0)$ (nm)	ℓ^{expt} (nm)	$\xi^{\text{expt}}(0)$ (nm)	$H_{c2}^c(0)$ (T)	$H_{c2}^{\text{expt}}(0)$ (T)
Cubic	2.4	2.08	15.2	0.71	4.4	22	18	4.7	3.9	3.1	2.6–3.3	3.3	32	29
Tetragonal	2.0	1.52	13.1	0.87	3.1	16	17	4.4	6.6	4.9	10.0	4.0	14	21
Cubic ^a	...	...	...	...	3.7	18	18	4.7	4.8	3.6	2.6–3.3	3.3	26	29

^aSame calculations as for the cubic phase, but after rescaling of the superconducting gap to match the experimental T_c .

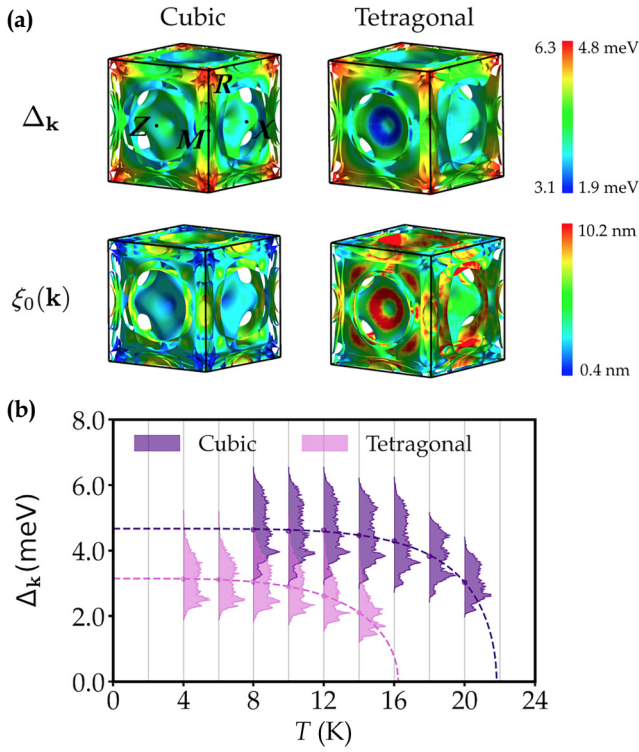


FIG. 6. (a) Distribution of the superconducting gap (top) and Pippard coherence length (bottom) over the Fermi surface at 8 K for the cubic (left) and tetragonal (right) phases of Nb₃Sn. The color scale indicates the magnitude of the superconducting gap $\Delta_{\mathbf{k}}$, ranging from its minimum value (blue) to its maximum value (red) across the Fermi surface of each phase, and the magnitude of the coherence length $\xi_0(\mathbf{k})$ ranging from the minimum value (0.4 nm) to the maximum value (10.2 nm) of the cubic phase. (b) Energy distribution of the zero-frequency superconducting gap of Nb₃Sn as a function of temperature, obtained by solving the anisotropic Migdal-Eliashberg equations using the full-bandwidth approach [26]. Dashed lines indicate a fit of the weighted averages of the distribution for each temperature.

pockets are composed mainly of transverse $d_{\perp}$ states from the Nb chains. The orbital distribution of the gap indicates a three-dimensional pairing mechanism that involves both longitudinal and transverse Nb orbitals, which challenges the traditional view that superconductivity in Nb₃Sn is driven by one-dimensional Nb chains. If pairing had involved only longitudinal states, the gap would be highly directional, with nodes or minima corresponding to off-chain states. Instead, the gap is broadly anisotropic but continuous, in agreement with most recent experiments.

The orbital character of the gap also explains why T_c is suppressed in off-stoichiometric or disordered samples, even when Nb chains remain structurally intact [2,54,58]: transverse $d_{\perp}$ states are particularly sensitive to local changes in the Sn environment, making Sn stoichiometry a key tuning parameter.

In tetragonal Nb₃Sn, the Fermi surface is slightly reshaped with noticeable changes in both Fermi velocity and gap distributions. In particular, the large-gap sheets near the R points lose spectral weight, while the two portions of the Fermi surface coming from the electron pockets around the Γ point show an increased Fermi velocity and reduced gap in the tetragonal direction around the Z points.

The temperature dependence of the superconducting gaps is shown in Fig. 6(b). Isotropic and anisotropic solutions both yield nearly identical critical temperatures for the two phases. Use of $\mu^* = 0.17$ extracted from the simple random-phase approximation yields a too-high T_c for the cubic phase ($T_c = 25$ K) compared with the experimental value ($T_c^{\text{expt}} = 18.3$ K). If we use the Kukkonen-Overhauser value ($\mu^* = 0.22$), we obtain theoretical T_c values of 22 K for the cubic phase and 16 K for the tetragonal phase, in much closer agreement with experimental values. While the cubic T_c is still slightly overestimated, the error is within the typical 10%–20% uncertainty of *ab initio* methods [59] and the calculated BCS ratios $2\Delta/k_B T_c$, reported in Table II, fall nicely within the experimental range of 4.2–4.9 [60].

B. Critical fields

Having access to the momentum-dependent solution of the ME equations, we can compute the momentum-resolved Pippard coherence length $\xi_0(\mathbf{k})$:

$$\xi_0(\mathbf{k}) = \frac{\hbar v_F(\mathbf{k})}{\pi Z_{\mathbf{k}} \Delta_{\mathbf{k}}}, \quad Z_{\mathbf{k}} = 1 + \lambda_{\mathbf{k}}. \quad (1)$$

In this expression, the Fermi velocities are renormalized by the normal-state self-energy $Z_{\mathbf{k}}$ to account for strong-coupling corrections [60]. The distribution of $\xi_0(\mathbf{k})$ over the Fermi surface is shown in Fig. 6(a), together with that of the superconducting gap. We find that the anisotropy of $\xi_0(\mathbf{k})$ is controlled mainly by the renormalized Fermi velocity $v_F^* = v_F/Z$, rather than directly by the gap: both small-gap and large-gap regions give rise to small ξ_0 if $v_F^*(\mathbf{k})$ is small. In the cubic phase, the electron pockets near the Γ point are small- ξ_0 regions due to their low $v_F(\mathbf{k})$ —see also Fig. S5 in Supplemental Material [39]. After the martensitic transition, i.e., in the tetragonal phase, these pockets become large- ξ_0 regions: along the tetragonal Z direction, $v_F(\mathbf{k})$ increases, while $\lambda_{\mathbf{k}}$ and $\Delta_{\mathbf{k}}$ decrease.

Using the calculated ξ_0 , we can obtain a fully *ab initio* estimate of the zero-temperature upper critical field $H_{c2}(T = 0)$. We do this by averaging $\xi_0(\mathbf{k})$ over the Fermi surface to extract an effective Ginzburg-Landau coherence length $\xi(0)$. The upper critical field can then be obtained as

$$H_{c2}(0) = \frac{\phi_0}{2\pi \xi^2(0)}, \quad \phi_0 = 2.068 \times 10^{-15} \text{ T m}^2, \quad (2)$$

where ϕ_0 is the magnetic flux quantum. In the clean limit, $\xi^c(0) \approx 0.74 \xi_0$ [61], which implies $H_{c2}^c(0) \propto 1/\xi_0^2$. Therefore, an increase in the average coherence length reduces the upper critical field. We find that $\langle \xi_0 \rangle$ increases from 3.9 nm in the cubic phase to 6.6 nm in the tetragonal phase, consistent with the observed suppression of H_{c2} during the martensitic transition. Our clean-limit estimates are $H_{c2}^c(0) = 32$ T for the cubic phase and $H_{c2}^c(0) = 14$ T for the tetragonal phase. The clean limit is valid when $\xi_0 \ll \ell$, where ℓ denotes the electronic mean free path. However, typical Nb_3Sn samples lie in the intermediate-to-dirty domain ($\xi_0 \sim \ell$), with ℓ^{expt} ranging from 2.6 nm in cubic samples to 10 nm in tetragonal samples [54,60]. In this regime, the mean free path reduces the effective coherence length [61]. Therefore, our clean-limit estimates should be regarded as lower bounds for $H_{c2}(0)$.

The calculated upper critical field for the cubic phase exceeds the experimental value $H_{c2}^{\text{expt}}(0) = 29$ T by approximately 10%. However, we observe that also T_c —and hence Δ —is larger than in experiments. If we rescale the gap and the T_c value, keeping $2\Delta/k_B T_c$ fixed (the bottom row in Table II), the estimate for $H_{c2}^c(0)$ improves to 26 T, which now lies below the experimental value and represents a consistent lower bound. For the tetragonal phase, on the other hand, the clean limit prediction of 14 T underestimates the experimental 21 T by approximately 50% [62]. Thus, we find that clean-limit formulas work reasonably well for samples in the clean-to-intermediate limit, where H_{c2} is still dominated by Fermi surface effects. This allows us to speculate about possible mechanisms for tuning the superconducting properties of A15 Nb_3Sn samples.

In particular, on the basis of our findings, we can provide a clear picture of how different doping strategies affect superconducting performance. Substitutional dopants introduce additional scattering, which drives the system toward the dirty limit and thereby increases H_{c2} while enhancing flux pinning and increasing J_c . Beyond this common effect, the impact of different types of impurity depends on which electronic states are modified. Doping on Sn sites may enhance the electron-phonon coupling of transverse $d_\perp$ states, which correspond to small-gap, large- ξ_0 regions. Strengthening these states would reduce anisotropy and simultaneously increase T_c and H_{c2} . This is consistent with reports that doping Sn sites with Al above 6% suppresses the structural transition and increases T_c up to 18.5 K, the highest value observed in Nb_3Sn [63]. In contrast, doping Nb sites (e.g., with Ti, Ta, or Hf) affects primarily the longitudinal Nb d states, which involve the same bands that form the large-gap pockets at the R point, as well as the Fermi surface sheets with the largest coherence lengths. As these extended regions limit H_{c2} , Nb-site doping could reduce coherence lengths and thereby increase H_{c2} . However, since it also affects the large-gap states, it tends to suppress T_c [12]. An illustrative

comparison of the band structure and Fermi velocity distribution supporting this picture for Ti substitution on Nb sites is provided in Supplemental Material [39].

VI. CONCLUSIONS

In this work, we presented a fully *ab initio* microscopic description of the superconducting state of Nb_3Sn , one of the workhorse superconductors for high-field applications. Our goal was to provide a reliable theoretical foundation for understanding and optimizing its performance, something that remained out of reach for more than 60 years.

Our results address three key open questions: (1) The martensitic transition in Nb_3Sn is not a second-order Peierls instability, but is a weakly first-order transition between two anharmonically stabilized structures. The tetragonal phase is never the global minimum of the potential energy surface in our calculations, but may be stabilized in real samples by internal stress. (2) The superconducting gap is single-valued but strongly anisotropic, in line with recent specific heat measurements [32,36]. (3) The martensitic transition suppresses the upper critical field H_{c2} , not simply because of the reduced coupling, but due to a redistribution of coherence lengths across the Fermi surface.

Beyond answering these questions, we uncovered several insights. We showed that accurately describing Nb_3Sn requires going beyond standard approximations in computational superconductivity. This work would not have been possible without recent community efforts to extend *ab initio* methods to real-world superconductors [64–68]. Harmonic phonon calculations—even with numerical artifacts such as increasing electronic smearing—fail to reproduce experimental phonon spectra. Anharmonicity, as observed for Nb-Ti and NbN [15,67], appears to be a general feature of real-world materials that is essential to stabilize the cubic and tetragonal structures. In addition, reproducing the experimental T_c values requires an advanced treatment of the Coulomb interaction beyond the empirical μ^* approximation and a full-bandwidth solution of the Migdal-Eliashberg equations.

Finally, we showed that the anisotropy of the superconducting gap arises from an unexpected three-dimensional pairing mechanism. Contrary to the traditional view [69], pairing is not limited to longitudinal $d_\parallel$ orbitals along the Nb chains, but also involves transverse $d_\perp$ orbitals with nearly equal weight. This leads to a strongly anisotropic single gap, consistent with experimental findings. The resulting coherence length $\xi_0(\mathbf{k})$ is controlled primarily by the renormalized Fermi velocity rather than by the gap amplitude. The martensitic transition reshapes the Fermi surface such that the Γ -centered electron pockets, which are small- ξ_0 ones in the cubic phase, become large- ξ_0 ones in the tetragonal phase. This

redistribution of coherence lengths increases the average ξ_0 and provides a microscopic explanation for the experimentally observed drop of H_{c2} across the martensitic transition.

These findings suggest practical strategies for optimizing Nb₃Sn performance. Doping of Sn sites may enhance the coupling on transverse orbitals and raise both T_c and H_{c2} , while also reducing gap anisotropy. Al doping is a promising candidate, having already shown the highest T_c in Nb₃Sn to date. Nb sites are usually doped with Ti, Ta, or Hf to prevent the martensitic transition and increase H_{c2} , despite lowering T_c [12]. Our results help explain this trade-off: doping directly on Nb sites affects the bands responsible for the large ξ_0 , reinforcing H_{c2} , but may also weaken the large-gap pockets at R points, leading to a drop in T_c . Even without chemical doping, it may be possible to prevent the martensitic transition by minimizing internal stress—e.g., by use of slower cooling rates or epitaxial growth—thereby maintaining higher superconducting performance. Although these strategies are rarely pursued, due to the difficulty of controlling Sn diffusion, epitaxial growth and thin-film deposition are actively studied in the context of superconducting radio-frequency cavities, where they have already shown excellent results.

This work represents an important step toward extending computational modeling to technologically relevant superconductors.

VII. METHODS

Electronic and vibrational properties were computed with DFPT within a plane-wave pseudopotential framework, as implemented in the QUANTUM ESPRESSO suite [70,71]. The plane-wave basis set used a kinetic energy cutoff of 80 Ry, ensuring convergence of the total energy to within 1 meV/atom. Scalar-relativistic optimized norm-conserving Vanderbilt pseudopotentials [72] were used in conjunction with the PBEsol exchange-correlation functional [38] for better agreement with experimental data. The structures were prerelaxed and then relaxed within the SSCHA. Structural relaxations were performed until the residual atomic forces were smaller than 2 meV/Å. Brillouin zone integrations were performed on a $12 \times 12 \times 12$ Γ -centered Monkhorst-Pack $\mathbf{k}$ -point mesh [73] with use of Methfessel-Paxton smearing of 0.005 Ry [74], and a $6 \times 6 \times 6$ $\mathbf{k}$ -point mesh for phonons [39].

To account for anharmonic effects in lattice dynamics, we used the SSCHA, as implemented in the SSCHA PYTHON package [25,75]. The initial guess for the force-constant matrix Φ was derived from DFPT dynamical matrices computed on 2^3 , 4^3 , and 6^3 $\mathbf{q}$ -point grids. The SSCHA minimization starts with a population of 200 individuals. The minimization process is then done with larger populations of 400 individuals. A final population of 13 000 individuals is used to extract the Hessian, which is more

sensitive to the number of configurations. The anharmonic phonon dispersions are obtained from the positional free-energy Hessians without the fourth-order term.

To access larger supercells and ensure convergence, we used moment tensor potentials [76], trained and evaluated with use of the MLIP package [77–79]. To train the potential, we generated a training set of 280 configurations and a validation set of 120 $2 \times 2 \times 2$ supercell configurations of the tetragonal phase, using the SSCHA code. To broaden the configurational sampling, the SSCHA temperature was set to 300 K during training. The moment tensor potential used eight radial basis functions with Chebyshev polynomials defined over the range [2.0 Å, 5.0 Å]. The potential accuracy was assessed by means of the root-mean-square error in energy with respect to DFT reference calculations on the validation set. After hyperparameter tuning, a level-24 potential was selected, yielding a root-mean-square error of 0.3 meV/atom.

To evaluate the superconducting properties of Nb₃Sn, we combined the fully anharmonic phonon spectra obtained from the SSCHA with electron-phonon matrix elements computed via DFPT. These matrix elements were calculated on coarse $\mathbf{q}$ -point and $\mathbf{k}$ -point grids and interpolated onto dense meshes with the use of Wannier functions, following the EPW method [55]. We performed interpolation to $36^3/72^3$ and $18^3/52^3$ fine meshes for the cubic phase and the tetragonal phase, respectively.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [80], embargo periods may apply.

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- [1] D. Larbalestier, A. Gurevich, D. M. Feldmann, and A. Polyanskii, High- T_c superconducting materials for electric power applications, *Nature* **414**, 368 (2001).
 - [2] A. Godeke, A review of the properties of Nb₃Sn and their variation with A15 composition, morphology and strain state, *Supercond. Sci. Technol.* **19**, R68 (2006).

- [3] C. Yao and Y. Ma, Superconducting materials: Challenges and opportunities for large-scale applications, *iScience* **24**, 102541 (2021).
- [4] G. Stewart, Superconductivity in the A15 structure, *Phys. C: Supercond. Appl.* **514**, 28 (2015).
- [5] D. Dew-Hughes, Superconducting A-15 compounds: A review, *Cryogenics* **15**, 435 (1975).
- [6] G. Shirane and J. D. Axe, Neutron scattering study of the lattice-dynamical phase transition in Nb_3Sn , *Phys. Rev. B* **4**, 2957 (1971).
- [7] R. N. Bhatt and W. L. McMillan, Landau theory of the martensitic transition in A-15 compounds, *Phys. Rev. B* **14**, 1007 (1976).
- [8] Y. Fujii, J. B. Hastings, M. Kaplan, G. Shirane, Y. Inada, and N. Kitamura, Study of the tetragonal-to-tetragonal phase transition of the A15 pseudobinary alloy $\text{Nb}_3\text{Sn}_{1-x}\text{Sb}_x$ by neutron and x-ray scattering, *Phys. Rev. B* **25**, 364 (1982).
- [9] L. R. Testardi, Structural instability and superconductivity in A-15 compounds, *Rev. Mod. Phys.* **47**, 637 (1975).
- [10] K. Tachikawa, H. Sekine, and Y. Iijima, Composite-processed Nb_3Sn with titanium addition to the matrix, *J. Appl. Phys.* **53**, 5354 (1982).
- [11] R. Flükiger, C. Senatore, M. Cesaretti, F. Buta, D. Uglietti, and B. Seeber, Optimization of Nb_3Sn and MgB_2 wires, *Superconductor Science and Technology* **21**, 054015 (2008).
- [12] S. M. Heald, C. Tarantini, P. J. Lee, M. D. Brown, Z. Sung, A. K. Ghosh, and D. C. Larbalestier, Evidence from EXAFS for different Ta/Ti site occupancy in high critical current density Nb_3Sn superconductor wires, *Sci. Rep.* **8**, 4798 (2018).
- [13] C. Tarantini, F. Kametani, S. Balachandran, S. M. Heald, L. Wheatley, C. R. M. Grovenor, M. P. Moody, Y.-F. Su, P. J. Lee, and D. C. Larbalestier, Origin of the enhanced Nb_3Sn performance by combined Hf and Ta doping, *Sci. Rep.* **11**, 17845 (2021).
- [14] L. Boeri, R. Hennig, P. Hirschfeld, G. Profeta, A. Sanna, E. Zurek, W. E. Pickett, M. Amsler, R. Dias, M. I. Eremets *et al.*, The 2021 room-temperature superconductivity roadmap, *J. Phys.: Condens. Matter* **34**, 183002 (2022).
- [15] A. Cucciari, D. Naddeo, S. Di Cataldo, and L. Boeri, NbTi: A nontrivial puzzle for the conventional theory of superconductivity, *Phys. Rev. B* **110**, L140502 (2024).
- [16] B. Sadigh and V. Ozoliņš, Structural instability and electronic excitations in Nb_3Sn , *Phys. Rev. B* **57**, 2793 (1998).
- [17] B. M. Klein and Z. Lu, Structural instabilities in A15 materials driven by anharmonic phonons: A first-principles study, *Phys. B: Condens. Matter* **296**, 120 (2001).
- [18] H. M. Tütüncü, G. P. Srivastava, S. Bağcı, and S. Duman, Theoretical examination of whether phonon dispersion in Nb_3Sn is anomalous, *Phys. Rev. B* **74**, 212506 (2006).
- [19] G. De Marzi, L. Morici, L. Muzzi, A. della Corte, and M. Buongiorno Nardelli, Strain sensitivity and superconducting properties of Nb_3Sn from first principles calculations, *J. Phys.: Condens. Matter* **25**, 135702 (2013).
- [20] R. Zhang, P. Gao, X. Wang, and Y. Zhou, First-principles study on elastic and superconducting properties of Nb_3Sn and Nb_3Al under hydrostatic pressure, *AIP Adv.* **5**, 107233 (2015).
- [21] F. Gala, G. De Marzi, L. Muzzi, and G. Zollo, The role of stoichiometry in superconducting $\text{Nb}_{1-\beta}\text{Sn}_\beta$: Electronic and vibrational properties from ab initio calculations, *Phys. Chem. Chem. Phys.* **18**, 32840 (2016).
- [22] X. Yang, Q. Du, L. Qiao, G. Xiao, Z. Li, and L. Yang, Microscopic origin of the abnormal elastic behavior accompanying the superconducting transition in Nb_3Sn crystals: An extended ab initio study, *J. Alloys Compd.* **941**, 168891 (2023).
- [23] L.-N. Wu, S.-T. Yang, J.-K. Shen, J.-S. Zhang, and F.-H. Liu, Coexistence of superconductivity and charge density wave instability in A15- Nb_3Sn , *Phys. Chem. Chem. Phys.* **25**, 32452 (2023).
- [24] W. Chen, X. Chen, Y. Gao, Y. Zhou, S. Cai, J. Zhao, K. Yang, A. Li, S. Jiang, Q. Wu *et al.*, Evolution of superconductivity and corresponding electronic structure in pressurized Nb_3Sn , *Superconductivity* **13**, 100153 (2025).
- [25] L. Monacelli, R. Bianco, M. Cherubini, M. Calandra, I. Errea, and F. Mauri, The stochastic self-consistent harmonic approximation: Calculating vibrational properties of materials with full quantum and anharmonic effects, *J. Phys. Condens. Matter* **33**, 363001 (2021).
- [26] R. Lucrezi, P. P. Ferreira, S. Hajinazar, H. Mori, H. Paudyal, E. R. Margine, and C. Heil, Full-bandwidth anisotropic Migdal–Eliashberg theory and its application to superhydrides, *Commun. Phys.* **7**, 33 (2024).
- [27] P. Ferreira, R. Lucrezi, I. Guilhon, M. Marques, L. Teles, C. Heil, and L. Eleno, Ab initio modeling of superconducting alloys, *Mater. Today Phys.* **48**, 101547 (2024).
- [28] P. W. Anderson and E. I. Blount, Symmetry considerations on martensitic transformations: “Ferroelectric” metals? *Phys. Rev. Lett.* **14**, 217 (1965).
- [29] B. W. Batterman and C. S. Barrett, Crystal structure of superconducting V_3Si , *Phys. Rev. Lett.* **13**, 390 (1964).
- [30] L. Vieland and A. Wicklund, Specific heat and the lattice transformation in Nb_3Sn , *Solid State Commun.* **7**, 37 (1969).
- [31] R. Mailfert, B. Batterman, and J. Hanak, Low temperature structural transformation in Nb_3Sn , *Phys. Lett. A* **24**, 315 (1967).
- [32] R. Escudero, F. Morales, and S. Bernès, Specific heat studies of pure Nb_3Sn single crystals at low temperature, *J. Phys.: Condens. Matter* **21**, 325701 (2009).
- [33] M. Acosta-Alejandro, J. Lezama-Pacheco, R. Falconi, R. Escudero, and J. Mustre de León, Local structure instability across the martensitic transition in Nb_3Sn , *J. Supercond. Novel Magn.* **24**, 1219 (2011).
- [34] V. Guritanu, W. Goldacker, F. Bouquet, Y. Wang, R. Lortz, G. Goll, and A. Junod, Specific heat of Nb_3Sn : The case for a second energy gap, *Phys. Rev. B* **70**, 184526 (2004).
- [35] M. Marz, G. Goll, W. Goldacker, and R. Lortz, Second superconducting energy gap of Nb_3Sn observed by breakjunction point-contact spectroscopy, *Phys. Rev. B* **82**, 024507 (2010).
- [36] Y. J. Jo, J. Zhou, Z. H. Sung, P. J. Lee, and D. C. Larbalestier, Specific heat of Nb_3Sn : The case for a single gap, *APL Mater.* **2**, 106101 (2014).
- [37] J. Zhou, Y. Jo, Z. Hawn Sung, H. Zhou, P. J. Lee, and D. C. Larbalestier, Evidence that the upper critical field of Nb_3Sn is independent of whether it is cubic or tetragonal, *Appl. Phys. Lett.* **99**, 122507 (2011).

- [38] J. P. Perdew, A. Ruzsinszky, G. I. Csonka, O. A. Vydrov, G. E. Scuseria, L. A. Constantin, X. Zhou, and K. Burke, Restoring the density-gradient expansion for exchange in solids and surfaces, *Phys. Rev. Lett.* **100**, 136406 (2008).
- [39] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/dmwh-1sbf> for further computational details on the *ab initio* calculations, as well as additional figures for convergence tests, electronic structure and Fermi-surface analysis, SSCHA convergence, and MLIP training.
- [40] S. Schickltanz, R. Kaiser, E. Schneider, and W. Gläser, Raman studies of A15 compounds, *Phys. Rev. B* **22**, 2386 (1980).
- [41] P. Jin, L. Li, X. Li, Q. Wang, and J. Cheng, Residual stress in Nb₃Sn superconductor strand introduced by structure and stoichiometric distribution after heat treatment, *IEEE Trans. Appl. Supercond.* **27**, 1 (2017).
- [42] J. Lee, S. Posen, Z. Mao, Y. Trenikhina, K. He, D. L. Hall, M. Liepe, and D. N. Seidman, Atomic-scale analyses of Nb₃Sn on Nb prepared by vapor diffusion for superconducting radiofrequency cavity applications: A correlative study, *Supercond. Sci. Technol.* **32**, 024001 (2019).
- [43] It is worth noting that the energy differences involved are so small that we cannot exclude the possibility that other effects could reshape the Born-Oppenheimer surface and stabilize a tetragonal phase. Indeed, test calculations using the PBE0 hybrid functional [81] predict a larger energy gain (approximately 5 meV/atom) for the experimental tetragonal structure over the cubic phase, at least at the harmonic level.
- [44] L. Boeri, G. Bachelet, E. Cappelluti, and L. Pietronero, Small Fermi energy and phonon anharmonicity in MgB₂ and related compounds, *Phys. Rev. B* **65**, 214501 (2002).
- [45] J. D. Axe and G. Shirane, Inelastic-neutron-scattering study of acoustic phonons in Nb₃Sn, *Phys. Rev. B* **8**, 1965 (1973).
- [46] L. Pintschovius, H. G. Smith, N. Wakabayashi, W. Reichardt, W. Weber, G. W. Webb, and Z. Fisk, Lattice dynamics of the A15 compound Nb₃Sb, *Phys. Rev. B* **28**, 5866 (1983).
- [47] L. Pintschovius, H. Takei, and N. Toyota, Phonon anomalies in Nb₃Sn, *Phys. Rev. Lett.* **54**, 1260 (1985).
- [48] L. Y. L. Shen, Tunneling into a high - T_c superconductor-Nb₃Sn, *Phys. Rev. Lett.* **29**, 1082 (1972).
- [49] D. A. Rudman and M. R. Beasley, Microscopic superconducting parameters from tunneling in A15 Nb-Sn, *Phys. Rev. B* **30**, 2590 (1984).
- [50] J. K. Freericks, A. Y. Liu, A. Quandt, and J. Geerk, Non-constant electronic density of states tunneling inversion for A15 superconductors: Nb₃Sn, *Phys. Rev. B* **65**, 224510 (2002).
- [51] G. Kieselmann and H. Rietschel, On the analysis of tunneling data for A15 superconductors, *J. Low Temp. Phys.* **46**, 27 (1982).
- [52] E. L. Wolf, *Principles of Electron Tunneling Spectroscopy* (Oxford University Press, 2011), ISBN: 9780199589494.
- [53] J. Geerk, U. Schneider, W. Bangert, H. Rietschel, F. Gompf, M. Gurvitch, J. Remeika, and J. Rowell, Electron tunneling into A15 and B1 superconductors, *Phys. B+C* **135**, 187 (1985).
- [54] M. Mentink, M. Dhalke, D. Dietderich, A. Godeke, F. Hellman, and H. T. Kate, The effects of disorder on the normal state and superconducting properties of Nb₃Sn, *Supercond. Sci. Technol.* **30**, 025006 (2017).
- [55] H. Lee, S. Poncé, K. Bushick, S. Hajinazar, J. Lafuente-Bartolome, J. Leveillee, C. Lian, J.-M. Lihm, F. Macheda, H. Mori *et al.*, Electron-phonon physics from first principles using the EPW code, *npj Comput. Mater.* **9**, 156 (2023).
- [56] P. Morel and P. W. Anderson, Calculation of the superconducting state parameters with retarded electron-phonon interaction, *Phys. Rev.* **125**, 1263 (1962).
- [57] C. Pellegrini, C. Kukkonen, and A. Sanna, Ab initio calculations of superconducting transition temperatures: When going beyond RPA is essential, *Phys. Rev. B* **108**, 064511 (2023).
- [58] J. P. Charlesworth, I. Macphail, and P. E. Madsen, Experimental work on the niobium-tin constitution diagram and related studies, *J. Mater. Sci.* **5**, 580 (1970).
- [59] A. Sanna, C. Pellegrini, and E. K. U. Gross, Combining Eliashberg theory with density functional theory for the accurate prediction of superconducting transition temperatures and gap functions, *Phys. Rev. Lett.* **125**, 057001 (2020).
- [60] T. P. Orlando, E. J. McNiff, S. Foner, and M. R. Beasley, Critical fields, Pauli paramagnetic limiting, and material parameters of Nb₃Sn and V₃Si, *Phys. Rev. B* **19**, 4545 (1979).
- [61] E. Helfand and N. R. Werthamer, Temperature and purity dependence of the superconducting critical field, H_{c2} . II, *Phys. Rev.* **147**, 288 (1966).
- [62] Our calculations refer to ideal stoichiometric crystals and do not include extrinsic effects such as inhomogeneity or residual cubic domains, which may justify why the experimentally observed T_c reduction (typically 1 K) is much smaller than the correspondent H_{c2} reduction.
- [63] L. J. Vieland and R. W. Cohen, Study of Transition Temperature in Superconductors, Final Report NAS 8-21384 (RCA Laboratories, Princeton, New Jersey 08540, 1970) prepared for NASA under Contract No. NAS 8-21384, reporting period: 11 March 1968 to 10 March 1970.
- [64] C. Tresca, G. Profeta, G. Marini, G. B. Bachelet, A. Sanna, M. Calandra, and L. Boeri, Why mercury is a superconductor, *Phys. Rev. B* **106**, L180501 (2022).
- [65] N. S. Sitaraman, Z. Sun, B. L. Francis, A. C. Hire, T. Oseroff, Z. Baraissov, T. A. Arias, R. G. Hennig, M. U. Liepe, D. A. Muller, and M. K. Transtrum (Center for Bright Beams), Enhanced surface superconductivity of niobium by zirconium doping, *Phys. Rev. Appl.* **20**, 014064 (2023).
- [66] S. D. Cataldo, W. Cursio, and L. Boeri, Vacancy-controlled superconductivity in rock-salt carbides: Towards predictive modelling of real-world superconductors, *arXiv:2506.07768*.
- [67] E. Kogler, M. R. Sahoo, C.-N. Tsai, F. Jöbstl, R. Lucrezi, P. I. C. Cooke, B. Kunert, R. Resel, C. J. Pickard, M. N. Julian *et al.*, Vacancy-free cubic superconducting NbN enabled by quantum anharmonicity, *Commun. Mater.* **6**, 283 (2025).
- [68] D. Jones, A. Östlin, A. Chmeruk, F. Beiuşeanu, U. Eckern, L. Vitos, and L. Chioncel, Quasiparticle Fermi surfaces

- of niobium and niobium-titanium alloys at high pressure, *Phys. Rev. B* **111**, 165152 (2025).
- [69] W. Weber and L. F. Mattheiss, Electronic structure of tetragonal Nb₃Sn, *Phys. Rev. B* **25**, 2270 (1982).
- [70] S. Baroni, S. de Gironcoli, A. D. Corso, and P. Giannozzi, Phonons and related crystal properties from density-functional perturbation theory, *Rev. Mod. Phys.* **73**, 515 (2001).
- [71] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo *et al.*, QUANTUM ESPRESSO: A modular and open-source software project for quantum simulations of materials, *J. Phys.: Condens. Matter* **21**, 395502 (2009).
- [72] D. R. Hamann, Optimized norm-conserving Vanderbilt pseudopotentials, *Phys. Rev. B* **88**, 085117 (2013).
- [73] H. J. Monkhorst and J. D. Pack, Special points for Brillouin-zone integrations, *Phys. Rev. B* **13**, 5188 (1976).
- [74] M. Methfessel and A. T. Paxton, High-precision sampling for Brillouin-zone integration in metals, *Phys. Rev. B* **40**, 3616 (1989).
- [75] I. Errea, M. Calandra, and F. Mauri, Anharmonic free energies and phonon dispersions from the stochastic self-consistent harmonic approximation: Application to platinum and palladium hydrides, *Phys. Rev. B* **89**, 064302 (2014).
- [76] I. Novoselov, A. Yanilkin, A. Shapeev, and E. Podryabinkin, Moment tensor potentials as a promising tool to study diffusion processes, *Comput. Mater. Sci.* **164**, 46 (2019).
- [77] R. Lucrezi, P. P. Ferreira, S. Hajinazar, H. Mori, H. Paudyal, E. R. Margine, and C. Heil, Full-bandwidth anisotropic Migdal–Eliashberg theory and its application to superhydrides, *Commun. Phys.* **7**, 33 (2024).
- [78] 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).
- [79] V. L. Deringer, M. A. Caro, and G. Csányi, Machine learning interatomic potentials as emerging tools for materials science, *Adv. Mater.* **31**, 1902765 (2019).
- [80] A. Cucciari and L. Boeri, Dataset supporting “An ab initio answer to long-debated questions about superconducting Nb₃Sn”, Zenodo, 2026, <https://doi.org/10.5281/zenodo.18226137>.
- [81] J. P. Perdew, M. Ernzerhof, and K. Burke, Rationale for mixing exact exchange with density functional approximations, *J. Chem. Phys.* **105**, 9982 (1996).