

Electron-phonon coupling and pairing mechanism in β -Bi₂Pd centrosymmetric superconductor

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We report first-principles calculations of the superconducting properties of β -Bi₂Pd within the fully anisotropic Migdal-Eliashberg formalism. We find a single anisotropic superconducting gap of s -wave symmetry which varies in magnitude on the different regions of the Fermi surface. The calculated superconducting energy gap on the Fermi surface, the superconducting transition temperature, the specific heat, and the quasiparticle density of states are in good agreement with the corresponding experimental results and support the view that β -Bi₂Pd is a phonon-mediated single-anisotropic-gap superconductor.

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I. INTRODUCTION

In recent years considerable attention has been devoted to the study of superconductors in the Bi-Pd family of alloys [1–4], in particular the noncentrosymmetric α -BiPd [5–8] and the centrosymmetric β -Bi₂Pd [9–17] compounds that have been found to exhibit topologically protected surface states with Rashba-like spin splitting. While the superconducting state of α -BiPd appears to be topologically trivial [6,7], the structure of the superconducting gap and the role of the topologically protected surface states in the superconducting pairing mechanism of β -Bi₂Pd still remain to be clarified. An early experimental study has suggested that β -Bi₂Pd is a multigap/multiband superconductor based on the temperature dependence of the electronic specific heat and the upper critical magnetic field data [9]. In contrast, recent scanning tunneling microscopy, calorimetric, Hall-probe magnetometry, muon spin relaxation, and point-contact spectroscopy measurements point towards a single s -wave superconducting gap [10–13]. Finally, while the absence of topological Andreev bound states in point-contact data [13] excludes the possibility of a topological superconducting behavior at the surface of β -Bi₂Pd, Majorana zero modes have been identified in β -Bi₂Pd crystalline films [14].

In this work, we present the first theoretical study of the phonons and the role of the electron-phonon interaction in the superconducting state of β -Bi₂Pd by performing state-of-the-art *ab initio* calculations powered by electron-phonon Wannier interpolation [18–20]. Since the strong spin-orbit coupling (SOC) inherent in the heavy-element Bi induces significant changes in the electronic band structure [15,16], the β -Bi₂Pd compound offers the opportunity to further study the interplay of the spin-orbit-coupling effect with superconductivity. We find that β -Bi₂Pd displays BCS-like superconductivity with a single anisotropic superconducting gap in agreement with recent experimental findings [10–13].

II. METHODOLOGY

The calculations are performed within the generalized gradient approximation to density-functional theory [21],

employing fully relativistic norm-conserving pseudopotentials [22,23], as implemented in the QUANTUM ESPRESSO suite [24]. The Perdew, Burke, and Ernzerhof (PBE) [25] form of the generalized gradient approximation was chosen to describe the exchange-correlation energy. The plane-wave kinetic-energy cutoff is 40 Ry. The Bi 6s²6p³ and Pd 4d⁹5s¹ orbitals were included as valence electrons. The β -Bi₂Pd phase crystallizes in the centrosymmetric body-centered tetragonal crystal structure with space group $I4/mmm$ (No. 139). To facilitate the comparison with the experimental results, we employ the experimental lattice constants ($a = 3.362$ Å and $c = 12.983$ Å [1]) for calculations without and with SOC [26]. A similar approach has been used in previous studies of superconductivity and charge-density-wave instability of other layered materials [27–30]. In both cases, the atomic positions were relaxed using a threshold of 10 meV/Å for the forces. The optimized internal parameter z_{Bi} for Bi atom is 0.361 (without SOC) and 0.362 (with SOC), which are in good agreement with the experimentally reported value of $z_{Bi} = 0.363$ [1]. The electronic charge density is calculated using an unshifted Brillouin zone (BZ) mesh with 12³ **k** points and a Methfessel-Paxton smearing of 0.02 Ry. The dynamical matrices and the linear variation of the self-consistent potential are calculated within density-functional perturbation theory [31] on the irreducible set of a regular 4³ **q**-point mesh.

The superconducting gap is evaluated using the anisotropic Migdal-Eliashberg formalism [32,33] as implemented in the EPW code [33–35]. We have recently used this methodology to investigate the superconducting properties of layered and two-dimensional materials with highly anisotropic Fermi surfaces [36–39]. The electronic wave functions required for the Wannier-Fourier interpolation [18,40] in EPW are calculated on a uniform unshifted Brillouin-zone grids of size 8³. Eleven maximally localized Wannier functions, three p states for each Bi atom and five d states for the Pd atom, are included to describe the electronic structure near the Fermi level. For the anisotropic Migdal-Eliashberg equations we use 90³ **k**-point and 45³ **q**-point grids. The Matsubara frequency cutoff is set to 7.5 times the largest phonon frequency, and the Dirac δ functions are replaced by Lorentzians with widths of 25 and 0.05 meV for electrons and phonons, respectively.

The technical details of the Migdal-Eliashberg calculations have been described extensively in Refs. [33,35]; here we only outline briefly the main procedure. In order to cal-

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culate the superconducting properties the fully anisotropic Migdal-Eliashberg equations are solved self-consistently along the imaginary axis at the fermion Matsubara frequencies $\omega_n = (2n + 1)\pi T$ (with n being an integer) for each temperature T :

$$Z(\mathbf{k}, i\omega_n) = 1 + \frac{\pi T}{N_F \omega_n} \sum_{\mathbf{k}'} \frac{\omega_{n'}}{\sqrt{\omega_{n'}^2 + \Delta^2(\mathbf{k}', i\omega_{n'})}} \times \delta(\epsilon_{\mathbf{k}'}) \lambda(\mathbf{k}, \mathbf{k}', n - n'), \quad (1)$$

$$Z(\mathbf{k}, i\omega_n) \Delta(\mathbf{k}, i\omega_n) = \frac{\pi T}{N_F} \sum_{\mathbf{k}'} \frac{\Delta(\mathbf{k}', i\omega_{n'})}{\sqrt{\omega_{n'}^2 + \Delta^2(\mathbf{k}', i\omega_{n'})}} \times \delta(\epsilon_{\mathbf{k}'}) [\lambda(\mathbf{k}, \mathbf{k}', -n') - \mu^*]. \quad (2)$$

$Z(\mathbf{k}, i\omega_n)$ is the mass renormalization function, $\Delta(\mathbf{k}, i\omega_n)$ is the superconducting gap function, $\lambda(\mathbf{k}, \mathbf{k}', n - n')$ is the momentum- and energy-dependent electron-phonon coupling, \mathbf{k} (\mathbf{k}') is an electronic state of combined band and momentum index, and μ^* is the semiempirical Coulomb parameter [41]. The anisotropic $\lambda(\mathbf{k}, \mathbf{k}', n - n')$ to be used in the Migdal-Eliashberg equations is given by

$$\lambda(\mathbf{k}, \mathbf{k}', n - n') = N_F \sum_{\mathbf{q}} \frac{2\omega_{\mathbf{q}}}{(\omega_n - \omega_{n'})^2 + \omega_{\mathbf{q}}^2} |g_{\mathbf{k}\mathbf{k}'}^{\mathbf{q}}|^2. \quad (3)$$

From the superconducting gap function $\Delta(\mathbf{k}, i\omega_n)$ one obtains the superconducting gap at real-valued frequencies $\Delta(\mathbf{k}, \omega)$ via Padé approximants [42,43]. The superconducting critical temperature T_c is identified as the temperature at which the leading edge $\Delta(\mathbf{k}, \omega = 0)$ of the superconducting gap vanishes.

III. ELECTRONIC AND VIBRATIONAL PROPERTIES

Figures 1(a) and 1(b) depict the decomposed band structure of β -Bi₂Pd along the main high-symmetry directions of the Brillouin zone [44] calculated without and with the inclusion of spin-orbit coupling. As previously reported [15,16], four bands of mixed orbital character cross the Fermi level. The two holelike bands centered around the Γ point originate from the Bi $6p_{x+y}/p_z$ orbitals, while the two electronlike bands along the Γ -X direction originate from the Bi $6p_{x+y}/p_z$ and Pd $4d_{xz+yz}/d_{xy}$ orbitals. These bands give rise to a complex multiple-sheet Fermi surface (FS) topology [16] that has been recently resolved using angular-resolved photoemission spectroscopy [15]. As shown in Figs. 1(c) and 1(d), the Fermi surface consists of a deformed two-dimensional cylindrical holelike sheet (FS2) enclosing a smaller hole pocket (FS1) centered around the Γ point. Surrounding the surface of the outer hole pocket, there is a three-dimensional electron pocket (FS3) which confines a second smaller electron pocket (FS4) along the Γ -X direction.

The inclusion of the SOC leads to the splitting of bands around the Fermi level and the opening of two continuous gaps that extend over the whole Brillouin zone, as shown in Fig. 1(b). As a result, the electronic density of states at the Fermi level N_F is increased by approximately 20%, from 0.659 to 0.788 state/[spin/(eV unit cell)]. Finally, there is a noticeable reduction in the size of the Γ -centered hole and electron pockets, although the Fermi surface topology remains unchanged with the inclusion of SOC.

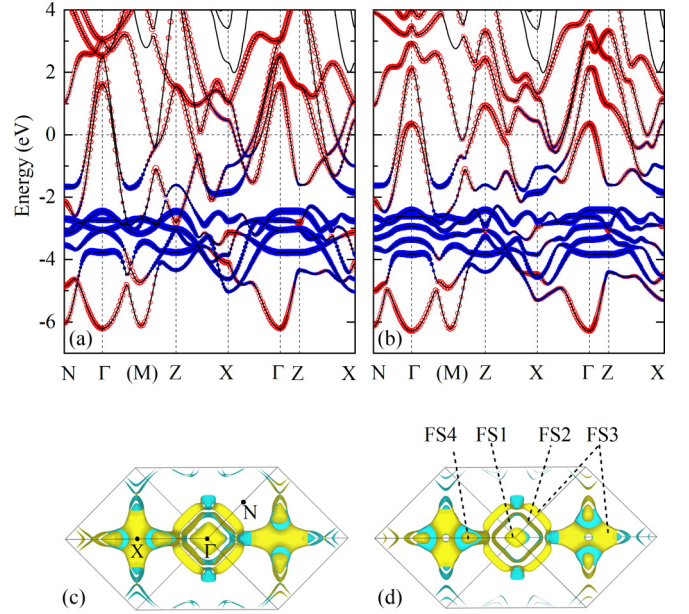


FIG. 1. Electronic band structure of bulk β -Bi₂Pd (a) without SOC and (b) with SOC. The size of the blue and red symbols is proportional to the contribution of Pd d and Bi p character. The corresponding Fermi surfaces are plotted in (c) and (d). The inner surface is shown in cyan, while the outer part is in yellow. The connection between the reciprocal lattice and the BZ is shown in Supplemental Fig. S1 [45]. The hole pockets are labeled as FS1 and FS2, and the electron pockets are labeled as FS3 and FS4.

In Figs. 2(a) and 2(b), we compare the phonon dispersion relations and the phonon density of states (PHDOS) calculated without and with SOC. In both cases, three regions can be clearly distinguished in the PHDOS: a low-energy region that extends up to 8.0 meV, an intermediate region from 8.0 to 10.0 meV, and a high-energy region above 10.0 meV. The decomposition of the phonon spectrum with respect to atomic vibrations is provided in Supplemental Fig. S2 [45]. The three acoustic phonon branches have a mixed character, with both types of atoms involved in the lattice vibration. That also holds for the first two optical branches. The higher optical phonons stem mostly from the vibration of Pd atoms, consistent with their lighter mass. The phonon spectrum changes only slightly with the inclusion of SOC. The frequencies of the highest optical modes are pushed upward by about 0.36 meV (2.5%) across the whole BZ, while the lowest acoustic branch softens along the Γ -Z direction.

In order to quantify the interaction between electrons and phonons, we calculate the Eliashberg spectral function $\alpha^2 F(\omega)$ and the cumulative electron-phonon-coupling (EPC) strength $\lambda(\omega)$. As shown in Fig. 2(c), the Eliashberg spectral function follows the trend of the PHDOS and exhibits a similar peak structure. Although the phonons from all energy regions contribute to the total EPC, the relative contributions of each set of modes differ considerably. The low-energy modes (up to 8.0 meV) account for approximately 60% of the total coupling ($\lambda = 0.77$), while the phonons in the intermediate- and high-energy regions have less sizable contributions of 22% and 18%, respectively. With inclusion of SOC, λ increases by 26% to

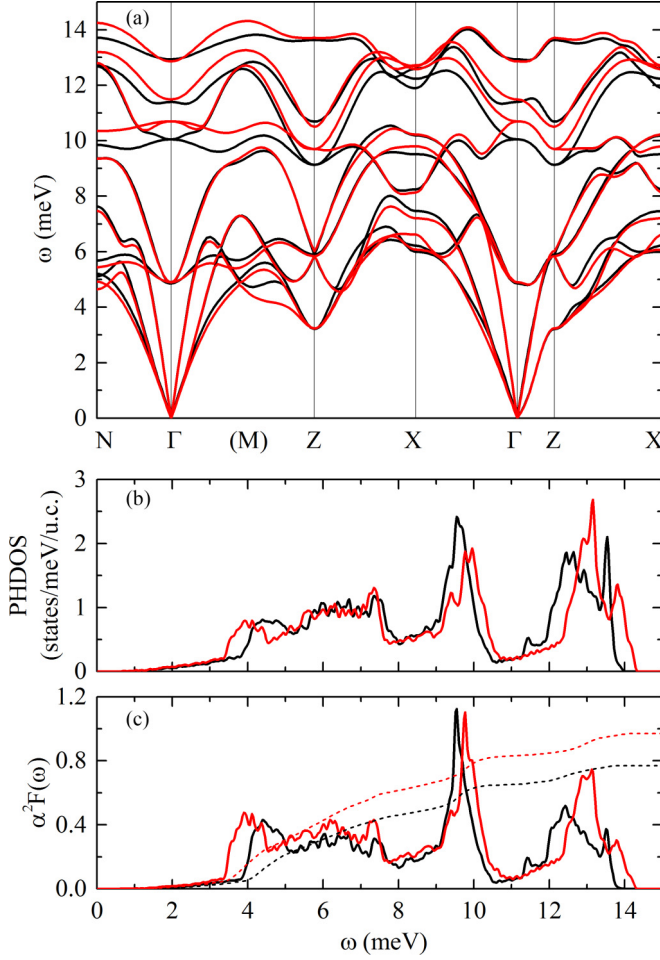


FIG. 2. (a) Phonon dispersion relations and (b) phonon density of states of β -Bi₂Pd. (c) Isotropic Eliashberg spectral function $\alpha^2 F(\omega)$ (solid line) and cumulative electron-phonon coupling strength $\lambda(\omega)$ (dashed line). The data without and with SOC are presented in black and red, respectively.

0.97. The SOC-induced enhancement of λ correlates with the increased density of states at the Fermi level and the softening of the low-energy phonon modes. In particular, the phonons in the low-energy region account for 0.15 of the total increase in λ , while the phonons in the intermediate- and high-energy regions only account for 0.01 and 0.04, respectively.

IV. SUPERCONDUCTING PROPERTIES

After assessing the EPC, we investigate its effect on the superconducting pairing mechanism. The superconducting gap function and the critical temperature are estimated by solving the anisotropic Migdal-Eliashberg equations [32,33,35]. Figures 3(a) and 3(b) show the energy distribution of the superconducting gap at the Fermi level as a function of temperature calculated without and with SOC and for a typical Coulomb pseudopotential $\mu^* = 0.1$. We find that β -Bi₂Pd exhibits an anisotropic single-gap structure characterized by a relatively broad energy profile with a spread of 0.38 meV (without SOC) and 0.34 meV (with SOC). The average value of the gap at zero temperature is estimated to be

$\Delta(0) = 0.65$ meV (without SOC) and $\Delta(0) = 0.70$ meV (with SOC). These values are in good agreement with scanning tunneling microscopy and muon-spin-relaxation measurements, yielding 0.76 [10] and 0.78 meV [12], respectively. Slightly larger values of 0.88 and 0.92 meV were reported based on calorimetric and Hall-probe magnetometry measurements [11,46] in the first case and point-contact spectroscopy measurements [13] in the second case. It is noteworthy that scanning tunneling measurements performed on the same samples as those used for the calorimetric and Hall-probe magnetometry measurements returned a superconducting gap in the 0.77–0.82 meV range [11,47]. These differences in the experimental results still remain to be understood, with one possible cause being the surface proximity effect [11]. Based on the Migdal-Eliashberg results, the superconducting gap vanishes at a critical temperature $T_c = 4.40$ K (without SOC) and $T_c = 4.55$ K (with SOC), close to the lower limit of the reported experimental values ranging from 4.25 to 5.4 K [1,2,9–13,15]. In order to test the sensitivity of our results to the parameters entering in the Migdal-Eliashberg equations, we have repeated the calculations for different electron and phonon meshes, smearing values, and Matsubara frequency cutoffs. The superconducting gap and critical temperature are found to be converged within 5%.

Figures 3(c) and 3(d) show the superconducting gap at 1 K on different parts of the Fermi surface. The same figures under three different perspectives are shown in Supplemental Fig. S3 [45]. We can clearly see that the gap opens on both the electron and hole pockets, and the magnitude of the gap changes greatly on some of the Fermi surface sheets. An essentially isotropic distribution is observed on the Bi-dominated inner hole FS1 pocket and the central region of the three-dimensional electron FS3 sheet with mixed Bi and Pd orbital character. On the contrary, the other parts of the Fermi surface display a strong anisotropy; in particular, the nearly cylindrical FS2 sheet shows the largest spread in $\Delta_{\mathbf{k}}$. Although the topology of the superconducting gap on the Fermi surface is practically not modified by the inclusion of the SOC, there is a noticeable difference between the absolute value of the gap on the inner Fermi surface. In the latter case, the superconducting gap is no longer characterized by a small spread around the minimum value but around the average value of $\Delta_{\mathbf{k}}$. This change is likely driven by the softening of the lowest acoustic branch along the Γ -Z direction which involves mainly out-plane Bi_z phonons. The structure of the gap correlates closely with the variation of the electron-phonon-coupling strength on the individual Fermi surface sheets shown in Supplemental Fig. S4 [45].

We further fit the temperature dependence of the average value of the superconducting gap using the single-band BCS s -wave model [48] and the single-band α model [49]. In the first case, we obtain the temperature-dependent gap by solving numerically the BCS gap equation [48,50]

$$\int_0^{k_B \theta_D / \Delta(0)} \tanh \left(\frac{\alpha_{BCS} \tilde{E}}{2t} \right) \frac{d\tilde{E}}{\tilde{E}} = \ln \left[\frac{2k_B \theta_D}{\Delta(0)} \right], \quad (4)$$

with $\Delta(0)$ taken from our first-principles calculations. Here $\alpha_{BCS} = 1.764$, $t = T/T_c$ is the reduced temperature, $\tilde{E} = \epsilon/\Delta(0)$ is the normalized normal-state single-particle energy, $k_B \theta_D$ is the maximum phonon energy within the Debye

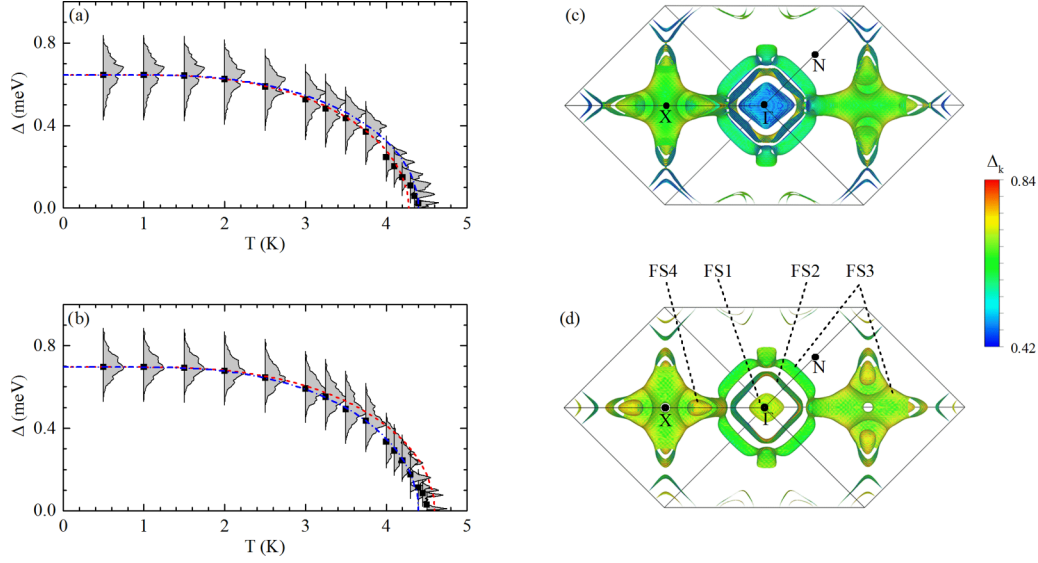


FIG. 3. Energy distribution of the anisotropic superconducting gap $\Delta_{\mathbf{k}}$ of β -Bi₂Pd as a function of temperature (a) without SOC and (b) with SOC. The gap is calculated using a Coulomb pseudopotential μ^* of 0.1. The black squares represent the average value of the gap, which vanishes at the critical temperature $T_c = 4.40$ K (without SOC) and 4.55 K (with SOC). The red dashed and blue dash-dotted lines are fits to the calculated data based on the BCS model and α model, respectively. Momentum-resolved superconducting gap $\Delta_{\mathbf{k}}$ (in meV) on the Fermi surface of β -Bi₂Pd at 1 K (c) without SOC and (d) with SOC.

theory set to 1000, $\tilde{E} = \sqrt{\tilde{\epsilon}^2 + \tilde{\Delta}^2}$ is the normalized excited quasiparticle (electron and hole) energy, and $\tilde{\Delta} = \Delta/\Delta(0)$ is the superconducting gap normalized by its zero-temperature value. In the second case, the data are fitted using the single-gap α model [49,50], which extends the BCS theory by introducing an adjustable parameter $\alpha = \Delta(0)/k_B T_c$. In this model the reduced gap $\tilde{\Delta}$ is assumed to be the same as in the BCS theory calculated from Eq. (4).

The results obtained with the two models are shown in Figs. 3(a) and 3(b) as red dashed and blue dash-dotted lines. Within the α model, the fitting parameters are found to be $\alpha = 1.71$ and $\alpha = 1.85$ for the calculations without and with SOC, respectively. All fitting curves give an overall good description of the temperature dependence of the superconducting gaps, although noticeable deviations can be seen in the region around the critical temperature. In particular, the two sets of *ab initio* data are best reproduced by the BCS model for calculations without SOC and by the α model for calculations with SOC, respectively.

In Fig. 4 we compare our results for the superconducting gap with the experimental data extracted from scanning tunneling microscopy [10] and point-contact spectroscopy [13] measurements. We find that both sets of experimental gaps are best fitted with the α model, similar to our SOC calculations. We obtain $\alpha = 1.90$ for the tunneling conductance data and $\alpha = 2.05$ for point-contact data. For comparison, the fits obtained with the BCS model display much larger deviations, as shown in Supplemental Fig. S5 [45]. The overall agreement between the theory and experiment is good; the temperature behavior of the superconducting gap (i.e., the shape of the curve) is almost perfectly reproduced. This can be more clearly seen in the inset in Fig. 4, where we plot the normalized superconducting gap $\Delta(T)/\Delta(0)$ versus the reduced temperature T/T_c .

Next, the temperature dependence of the normalized electronic specific heat in the superconducting state is calculated within the α model using the following expression [50]:

$$\frac{C_{es}(T)}{\gamma_n T_c} = \frac{6\alpha^3}{\pi^2 t} \int_0^\infty \left[f(1-f) \left(\frac{\tilde{E}^2}{t} - \frac{1}{2} \frac{d\tilde{\Delta}^2}{dt} \right) \right] d\tilde{\epsilon}, \quad (5)$$

where $f = [\exp(\alpha \tilde{E}/t) + 1]^{-1}$ is the Fermi-Dirac distribution function and $\gamma_n = (2/3)\pi^2 k_B^2 N_F$ is the Sommerfeld coefficient. The temperature derivative of the gap function

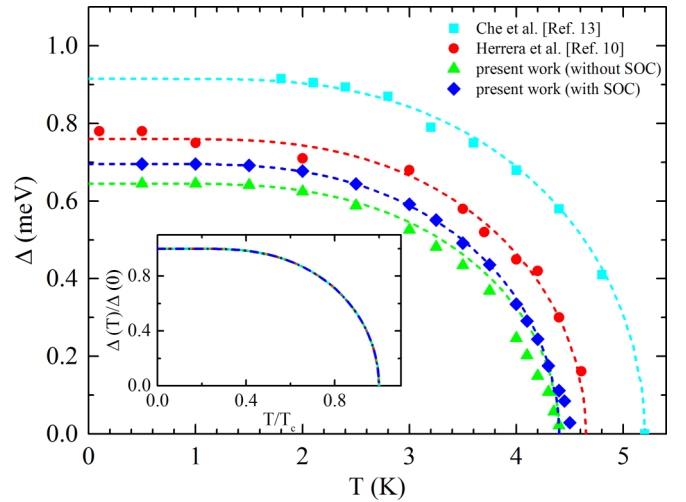


FIG. 4. Comparison between theoretical and experimental [10,13] superconducting gaps as a function of temperature. The theoretical data represent the average value of the gap extracted from Figs. 3(a) and 3(b). The curves are fits to the superconducting gap values within the α model.

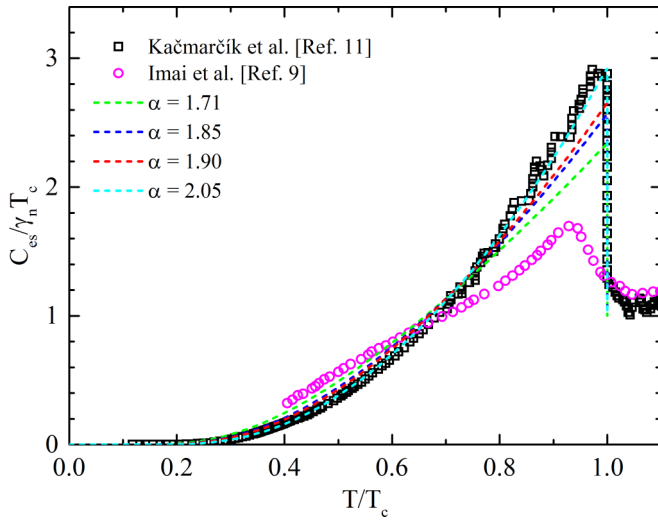


FIG. 5. Calculated and experimental normalized electronic specific heat as a function of T/T_c .

$d\tilde{\Delta}^2(t)/dt$ is given by [50]

$$\frac{d\tilde{\Delta}^2(t)}{dt} = \frac{\int_0^\infty \text{sech}^2(g)d\tilde{\epsilon}}{\int_0^\infty \left[\frac{t \text{sech}^2(g)}{2(\tilde{\epsilon}^2 + \tilde{\Delta}^2)} - \frac{t^2 \tanh(g)}{\alpha_{BCS}(\tilde{\epsilon}^2 + \tilde{\Delta}^2)^{3/2}} \right] d\tilde{\epsilon}}, \quad (6)$$

where $g = \frac{\alpha_{BCS}\sqrt{\tilde{\epsilon}^2 + \tilde{\Delta}^2}}{2t}$. In Fig. 5 we plot the reduced specific heat obtained from the temperature dependence of the superconducting gap corresponding to the four fits based on the α model in Fig. 4 together with the experimental data extracted from thermal-relaxation [9] and calorimetric [11] measurements. To facilitate the comparison, we renormalize the temperature to T_c , using the corresponding experimental and theoretical values. The normalization procedure for the experimental data is shown in Supplemental Fig. S6 [45]. The results for $\alpha < 2$ associated with the theoretical data (green and blue dashed lines) and scanning tunneling microscopy data (red dashed line) compare well over the whole temperature range. The discontinuity at the critical temperature $\Delta C_e/\gamma_n T_c = 1.426(\alpha/\alpha_{BCS})^2$ is found to be 1.34 (for $\alpha = 1.71$), 1.57 (for $\alpha = 1.85$), and 1.65 (for $\alpha = 1.90$), close to the BCS value of 1.43. A larger discrepancy is observed, particularly in the high-temperature region $t > 0.8$, when the results for $\alpha < 2$ are compared to the ones for $\alpha = 2.05$ associated with the point-contact data (cyan dashed line) and the calorimetric specific-heat measurements (black squares) [11]. In the latter two cases, the jump at the critical temperature is estimated to be 1.93. Despite the aforementioned differences, all these results give a specific-heat temperature dependence consistent with the one-gap BCS model. Moreover, they differ strikingly from the earlier specific-heat measurements (magenta circles), disproving the suggestion of multigap superconductivity [9].

The argument for a multigap scenario presented in Ref. [9] was based on the appearance of an additional hump in the specific heat at approximately 3 K, as shown in Supplemental Fig. S6(a). A similar low-temperature feature observed in the MgB_2 superconductor at approximately 10 K was caused by a second energy gap [51–53]. Under this assumption, a two-gap

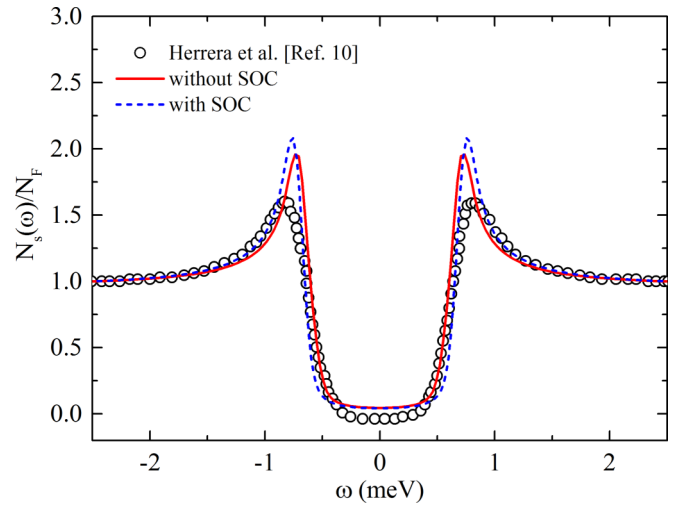


FIG. 6. Calculated normalized quasiparticle DOS in the superconducting state of Bi_2Pd without (red solid line) and with (blue dashed line) SOC compared to tunneling data from Ref. [10] (black circles) for $T = 1$ K.

model with energy gap parameters of 0.54 and 1.29 meV [54] was shown to reproduce well the temperature dependence of the measured specific heat [9]. However, it is noteworthy that in this case the energy value of the main gap is quite significantly larger than the latest reported results [10–13]. Moreover, Kačmarčík *et al.*'s [11] very detailed study of the specific-heat capacity could not find any sign of a second energy gap. Further comparison of the two sets of data reveals that the jump in the specific heat near the critical temperature is much broader in Ref. [9] compared to Ref. [11], pointing towards highly homogeneous Bi_2Pd single crystals in the latter case. It is then likely that the observed hump belongs to other Bi-Pd superconducting alloys and the x-ray diffraction pattern indeed shows the presence of a α - Bi_2Pd phase [9].

Besides the temperature dependence of the specific heat, other measurements have been used to address the issue of multigap superconductivity. The temperature dependence of the lower critical field [10–12] and the magnetic field dependence of the superconducting gap [13] were very well described by one-gap models providing additional support for a standard single s -wave superconducting gap.

Finally, we calculate the quasiparticle density of states (DOS) in the superconducting state $N_s(\omega)$ according to

$$\frac{N_s(\omega)}{N_F} = \text{Re} \left[\frac{\omega}{\sqrt{\omega^2 - \Delta^2(\omega)}} \right]. \quad (7)$$

Our results at 1 K are shown in Fig. 6 and compared directly to the experimental tunneling conductance of Ref. [10]. The superconducting DOS is scaled so that its high-energy tail coincides with the DOS in the normal state. The agreement between our calculations and experiment is very good, with all sets of data exhibiting two symmetric peaks characteristic of a single-gap structure.

V. CONCLUSIONS

In conclusion, we have studied the superconducting properties of β -Bi₂Pd within the *ab initio* anisotropic Migdal-Eliashberg theory. We have shown that the spin-orbit coupling results in only a slight increase in the predicted superconducting gap and critical temperature, while the structure of the superconducting gap remains practically unaffected. We find a sizable anisotropy in the electron-phonon coupling leading to a single superconducting gap which varies in magnitude over the disconnected sheets of the Fermi surface.

The experimental superconducting gap, critical temperature, specific heat, and tunneling conductance are well described assuming a conventional phonon-mediated mechanism as the origin of the superconducting transition.

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