Intermetallics 84 (2017) 136–141

Contents lists available at ScienceDirect

Intermetallics

journal homepage: www.elsevier.com/locate/intermet

Electron-phonon interaction and superconductivity in the multiband superconductor β-Bi_2Pd

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ARTICLE INFO

Article history:
Received 25 August 2016
Received in revised form
21 November 2016
Accepted 15 January 2017

Keywords:
Intermetallics
Density functional theory
Electronic structure
Superconducting properties
Ab initio calculations
Physical properties

ABSTRACT

We have investigated the structural, electronic, and vibrational properties of β-Bi_2Pd in the body-centered tetragonal CaC_2 structure using a generalized gradient approximation of the density functional theory and the *ab initio* pseudopotential method. There are several electronic bands near the Fermi energy, with varying degrees of dispersive behaviour, which arise dominantly from Bi 6p orbitals and also from Bi 5d and Pd 5p orbitals. A critical assessment of the Eliashberg spectral function reveals that Bi-related vibrations couple strongly with the electrons at the multiband Fermi energy. By integrating the Eliashberg spectral function, the values of the average electron-phonon coupling and the logarithmic average frequency are determined to be 1.03 and 79.23 K, respectively. With these values, the Allen-Dynes formula suggests the BCS superconducting transition temperature of $T_c = 5.5$ K, in excellent agreement with the recently presented experimental value of 5.4 K.

1. Introduction

Multiband superconductivity (MBSC) can be linked to the existence of separate pockets in the Fermi surface centered around some points of the Brillouin zone. Furthermore, MBSC may also appear in nanofilms made of common single-band superconducting compounds, where the geometrical size quantization generates apparent carrier subbands [1–3]. This unusual phenomenon was first found theoretically shortly after the development of the BCS theory [4]. Suhl and co-workers [4] offered a model for MBSC in transition metals by accounting for an overlap between s and d bands. Separately, Moscalenko [5] suggested an enlargement of the BCS theory for multiple bands. On the experimental side [6], MBSC was first observed for Nb-doped $SrTiO_3$. Two-band superconductivity was also found for the rare earth nickel borocarbides (RNi_2B_2C) [7]. Three decades of experimental observations of MBSC have received renewed interest due to the special properties of the 40 K superconductor MgB_2 [8], where the situation for two-band superconductivity is engrossing. Furthermore, a gap much smaller in MgB_2 than the expected BCS gap was analyzed in tunneling experiments [9]. The main consequence of small gap is the talent to handily excite quasi-particles, which can make the properties of this s-wave superconductor similar to those of a d-wave superconductor. After the discovery of MBSC in MgB_2, multiband impressions arising from multiple sheets of Fermi surface have been found in other kinds of superconductors, such as $MgCNi_3$ [10], iron-based superconductors [11], $NbSe_2$ [12] and $Lu_2Fe_3Si_5$ [13,14]. Furthermore, Takayama and co-workers [15] have reported the synthesis of a new family of ternary platinum phosphide superconductors with the chemical formula APt_3P (A = Sr, Ca and La) and the superconducting transition temperatures of 8.4, 6.6, and 1.5 K, respectively. Based on the observation of nonlinear temperature behavior of the Hall resistivity, Takayama and co-workers [15] indicate the existence of MBSC in these materials.

In 2012, Imai and co-workers [16] have investigated bulk superconductivity in a high-quality single crystal of Bi_2Pd (β-Bi_2Pd; space group: $I4/mmm$) with a superconducting transition temperature of 5.4 K, by examining its electrical resistivity, magnetic and specific heat. However, an early experimental work [17] disclosed that this compound depicted superconductivity at temperatures less than 4.25 K. This difference can be related to the high-quality

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http://dx.doi.org/10.1016/j.intermet.2017.01.009
0966-9795/

single crystal of Bi_2Pd in the recent experimental work of Imai and co-workers [16]. The temperature dependence of the upper critical magnetic field and specific heat reveal that β-Bi_2Pd is a multiple-gap superconductor [16]. Recently, Herrera and co-workers [18] have presented very low-temperature scanning tunneling microscopy experiments on single-crystalline samples of the superconductor β-Bi_2Pd. They find that the magnetic field dependence of the intervortex tunneling conductance is higher than the one expected in a single-gap superconductor [18]. Such an increase in the intervortex tunneling conductance can be seen in superconductors with multiple superconducting gaps. Very recently, the comprehensive calorimetric studies [19] via the sensitive ac technique have also indicated that β-Bi_2Pd is a single s-wave gap strong-coupled superconductor with $2\Delta/k_BT_c = 4.1$.

On the theoretical side, Shein and Ivanovskii [20] have studied the electronic band structure and Fermi surface of the body-centered tetragonal β-Bi_2Pd. They find that the density of states near the Fermi level is of a mixed character and is formed primarily by Pd 4d and Bi 6p states [20]. Furthermore, they show that the effect of spin-orbit coupling is of minor importance for the distribution of the near-Fermi electronic states [20]. In addition to this theoretical work [20], Sharma and co-workers [21] have studied the electronic and vibrational properties of the body-centered tetragonal β-Bi_2Pd. Electronic calculations in this work [21] have been performed by using the full-potential linearized augmented plane wave method and a generalized gradient approximation of the density functional theory, while phonon calculations have been carried out with the projector augmented wave method [21]. Their phonon calculations show that β-Bi_2Pd is dynamically unstable [21]. However, while they did not calculate the electron-phonon interaction for this compound, they estimated the electron-phonon coupling parameter to be a very large value of 3.66 from their low temperature specific heat measurements. Using their estimated value of the electron-phonon coupling parameter, they estimated the superconducting transition temperature of β-Bi_2Pd to be 23.08 K, which is more than four times higher than the experimental value of 5.4 K obtained by Imai and co-workers [16].

Although some theoretical investigations [20,21] of the structural, electronic and vibrational properties of β-Bi_2Pd have been carried out, no theoretical or established experimental results are available for the electron-phonon interaction in this material. However, it is well known that a number of important physical properties of metals is governed by the electron-phonon interaction. The electrical and thermal resistivities, superconductivity, softening of phonon modes, renormalization of the low-temperature electronic component of the heat capacity, and a number of other physical phenomena can be commented clearly only with the knowledge of the spectral distribution function of the electron-phonon interaction in each particular substance. The importance of electron-phonon interaction motivates us to examine structural, electronic, vibrational and electron-phonon interaction properties of β-Bi_2Pd. The structural and electronic properties are investigated by using the plane wave pseudopotential method within the generalized gradient approximation of the density functional scheme. We have also carried out *ab initio* linear response calculations of the lattice dynamics and polarization characteristics of zone-centre phonon modes. Furthermore, the linear response method [22] and the Migdal-Eliashberg approach [23,24] have been utilized to calculate the electron-phonon matrix elements. The Eliashberg spectral function is obtained from the calculated phonon spectrum and the calculated electron-phonon matrix elements. Furthermore, the average electron-phonon coupling parameter λ is calculated from the Eliashberg spectral function. Finally, an explanation for the difference in the superconducting transition temperature between the isostructural materials β-Bi_2Pd, YC_2 and LaC_2 [25] has been put forward.

2. Theory

Within the Migdal-Eliashberg theory of superconductivity [23,24], first-principles calculations [26,27] of superconducting properties need the knowledge of (i) the electronic structure, (ii) the phonon spectrum, and (iii) the electron-phonon matrix elements of the material. The first principles calculations presented in this work are carried out using the Quantum-Espresso program [22], which is based on the density functional theory, within the plane-wave pseudopotential method. The Kohn-Sham equations [28] are solved using the Perdew-Burke-Ernzorhof generalized gradient approximation (GGA) [29]. The electron-ion interaction is described by using norm-conserving pseudopotentials [30]. A basis set containing all plane waves up to the cut off energy of 60 Ry has been taken. A (8× 8× 8) zone-centred grid is used to obtain the structural parameters of β-Bi_2Pd. The electronic structure and the electronic density of states are obtained with a (24× 24× 24) zone-centred grid. The linear response method [22] is used to study the lattice dynamics by using the (8× 8× 8) zone-centred grid, giving 59 $\boldsymbol{k}$ points in the irreducible part of the Brillouin-zone. We estimate that phonon frequencies are accurate to within 0.1 THz for the present choice of kinetic energy cutoff and the special **k** points. We have calculated thirteen dynamical matrices which are Fourier transformed to achieve the full phonon spectrum and the vibrational density of states. Then, the phonon density of states and the electron-phonon matrix elements are then used to determine the Eliashberg spectral function from which the superconducting properties of the materials are obtained. Fermi-surface sampling for the evaluation of the electron-phonon matrix elements has been performed using 24× 24× 24 $\boldsymbol{k}$-mesh with a Gaussian width 0.001 Ry. The phonon density of states and the Eliashberg function are also determined using this $\boldsymbol{k}$-mesh. We have used the density functional theory in our calculations because this theory has proven to be one of the most accurate methods for the computation of the electronic structure of solids [31–36].

3. Results

3.1. Structural and electronic properties

The studied superconductor (β-Bi_2Pd) possesses the body-centered tetragonal CaC_2 structure, with space group $I4/mmm$, and one formula unit per primitive unit cell. The atomic configuration consists of two Bi atoms at the (4e) (0, 0, z_{Bi}), (0, 0,-z_{Bi}) positions and one Pd atom at the 2(a) (0, 0, 0) position. The starting value of z_{Bi} is taken to be 0.375. This structure can be schematically explained as a stacking of square layers of Bi and Pd in the sequence …Pd/Bi/Bi/Pd… along the z direction, as seen in Fig. 1. The *ab initio* calculations have been carried out to determine total energy results, which are then fitted into the Murnaghan equation of state [37] to obtain the structural parameters. The determined equilibrium lattice constants (a and c), the internal parameter (z_{Bi}), the nearest Bi-Pd distance (d_{Bi-Pd}), bulk modulus (B) and its pressure derivative (B') are presented in Table 1 along with the available experimental [16,17] and theoretical [20] results. In general, the calculated results compare very well with experimental [16,17] and previous theoretical results [20]. In particular, the determined lattice constants a and c vary from the recently measured values [16] within 1.7% and 2.0%, respectively, while the calculated internal parameter ($z_{Bi} = 0.365$) is slightly larger than its experimental value [17] of 0.363. The value of the Bi-Pd bond length is found to be 3.008 Å, which is slightly larger than the sum of the covalent radii of