Electron-phonon coupling in the magnetic Weyl semimetal ZrCo_2Sn

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(Received 23 September 2020; accepted 12 January 2021; published 25 January 2021)

Electron-phonon coupling in ZrCo_2Sn is investigated within the density-functional theory and linear-response approach in the mixed-basis pseudopotential representation. Phonon-induced scattering is analyzed for excited electrons (holes) in two majority bands, which form the topological Weyl state. Although the electron-phonon coupling in the energy range under consideration demonstrates some dependence on the available phase space, the strength of the phonon-mediated scattering, λ , changes rather weakly with the hole (electron) energy and momentum, varying between 0.1 and 0.3. The momentum-averaged value of λ ranges from 0.25 to 0.45. The phonon-mediated scattering of electrons near the Weyl point is found to be weak enough to warrant well-defined quasiparticles. Most of the modes actively involved in electron scattering are middle- and high-frequency lattice vibrations, while the participation of low-energy acoustic phonons is significantly suppressed by electron-phonon matrix elements. Of the long-wavelength optical phonons, only the T_{2g} Raman active modes generated by opposite vibrations of Co atoms make a noticeable contribution to the scattering of electrons.

DOI: [10.1103/PhysRevB.103.024303](https://doi.org/10.1103/PhysRevB.103.024303)

I. INTRODUCTION

Electron-phonon (e-ph) coupling (EPC) is one of the fundamental many-body processes that affect the lifetime of electron (hole) excitations [1] and, therefore, can be a limiting factor for applications of topological edge states at elevated temperatures. That is why the estimation of the strength of e-ph interaction in the metallic surface state of topological insulators has become of great importance [2–10]. A theoretical analysis based on first-principle calculations showed that the momentum-averaged EPC strength in the topological surface state of Bi_2Se_3 and Bi_2Te_3 is relatively low, $\lambda(E) < 0.15$, and essentially follows a linear increase in the density of electronic states with the distance from the Dirac (crossing) point [9]. Thus, phonon-mediated scattering was found to be weak enough to guarantee well-defined and long-lived quasiparticles even at room temperature. The main restricting factors responsible for such a weak e-ph interaction are that (i) only long-wavelength phonons can participate in EPC because of the small momentum range of the Dirac-like surface state; and (ii) the coupling is significantly suppressed by the peculiar spin texture of the topological state with the spin locked perpendicular to the momentum (spin helicity) [5,11].

Is the EPC also weak in materials with Weyl fermions, for example, in a family of Weyl semimetals? These compounds are characterized by the presence of intersections (Weyl

points) of nondegenerate energy bands that are topologically stable as long as they remain separated in momentum space. Since the touching bands should be nondegenerate, either the time reversal symmetry or the inversion must be broken [12]. An interesting type of Weyl semimetals with broken time reversal symmetry represents the magnetic Heusler compounds, where exotic transport properties are expected [13]. Unlike the time-reversal-invariant Weyl semimetals, which possess a substantial number of Weyl nodes [14–17], the magnetic Heusler compounds exhibit only two symmetry-related Weyl points, the minimal required number, whose energy position can be tuned to the Fermi level by alloying [13].

These Co(Ni)-based ferromagnets have attracted much attention because of not only their electronic, but also their magnetic properties [18–22]. A distinctive feature of these compounds is the bandgap in minority bands that arises around the Fermi level, which implies a half-metallic behavior with full spin polarization at E_F , where only the majority spins are present [23,24]. Two of the majority bands form a Weyl point along the magnetization direction, which is protected by the rotation symmetry [13].

In this article, we focus on one of the Co-based Heusler compounds, ZrCo_2Sn , and study the interaction of phonons and excited holes (electrons) in the energy gap, where there are several majority bands crossing E_F . Since phonon-mediated interband transitions are possible, the wavelength of phonons which can participate in the e-ph interaction is not restricted now to a small momentum range, as in topological

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insulators. The restriction associated with the spin texture of electronic states also does not exist. All the bands belong to the majority spin channel.

To clarify how the electronic states couple to phonons, we calculated the e-ph coupling constant for electrons (holes) with different momenta in the energy range from -0.2 to $+1.4$ eV relative to E_F . The data obtained are presented as energy and momentum resolved. In addition, to compare the coupling constant of a specific electronic state and the momentum-averaged value, we calculated the average strength of the electron-phonon interaction at energies from -0.1 to $+1$ eV. This also made it possible to estimate the effect of variations in the density of electronic states on the value of the e-ph constant.

The paper is organized as follows. In Sec. II a short outline of the calculation method is given. Section III contains a discussion of the calculated phonon dispersion and the phonon-mediated electron scattering. Finally, in Sec. IV the conclusions are drawn.

II. CALCULATION DETAILS

The e-ph coupling parameter for a hole (electron) state with momentum $\mathbf{k}$ and band index i is defined as [25]

$$\lambda_{\mathbf{k}i} = \int_0^{\omega_m} \lambda_{\mathbf{k}i}(\omega) d\omega = \int_0^{\omega_m} \frac{\alpha^2 F_{\mathbf{k}i}^{\text{em}}(\omega) + \alpha^2 F_{\mathbf{k}i}^{\text{ab}}(\omega)}{\omega} d\omega. \quad (1)$$

Here ω_m is the maximum phonon frequency. The electron-state-dependent Eliashberg spectral function corresponding to the phonon emission (em) and absorption (ab) processes is given by

$$\alpha^2 F_{\mathbf{k}i}^{\text{em/ab}}(\omega) = \sum_{\mathbf{q}, \nu, f} \delta(\epsilon_{\mathbf{k}i} - \epsilon_{\mathbf{k}+\mathbf{q}f} \mp \omega_{\mathbf{q}\nu}) \times |g_{\mathbf{k}+\mathbf{q}f}^{\mathbf{q}\nu}, \mathbf{k}i|^2 \delta(\omega - \omega_{\mathbf{q}\nu}). \quad (2)$$

Here $\epsilon_{\mathbf{k}i}$ and $\epsilon_{\mathbf{k}+\mathbf{q}f}$ are the energies of the initial and final electronic states, respectively, and $g_{\mathbf{k}+\mathbf{q}f}^{\mathbf{q}\nu}, \mathbf{k}i$ denotes the e-ph matrix elements that give the probability of scattering from initial state $\mathbf{k}i$ to final state $\mathbf{k} + \mathbf{q}f$ by phonon $\mathbf{q}\nu$ with frequency $\omega_{\mathbf{q}\nu}$. The minus and plus signs in the δ function correspond to phonon emission and absorption, respectively. The sum is carried out over all possible final electron states in the full three-dimensional Brillouin zone (BZ) and phonon modes. When $\lambda_{\mathbf{k}i}$ is averaged over all initial electron states at a fixed energy (E) one obtains the momentum-averaged strength of e-ph coupling, $\lambda(E)$ [26].

We performed scalar relativistic spin-polarized calculations within the framework of the density-functional theory using the mixed-basis pseudopotential approach. To represent valence states a combination of local functions and plane waves was employed [27,28]. The phonon dispersion was obtained using a linear response technique [29,30]. The norm-conserving pseudopotentials were constructed according to the scheme proposed by Vanderbilt [31] with semicore states included: s and p for Zr and Co and d for Sn. The exchange and correlation energy functional was evaluated within the generalized gradient approximation (GGA-PBE)

[32]. Using a kinetic energy cutoff of 24 Ry, integrations over the BZ were performed by sampling a $16 \times 16 \times 16$ $\mathbf{k}$ -point mesh [33] corresponding to 145 points in the irreducible wedge of the BZ, combined with a Gaussian broadening with a smearing parameter of 0.1 eV. Since e-ph matrix elements for a fixed electronic state display rather significant variations throughout the BZ, the summation over wave vectors requires a dense mesh of $\mathbf{q}$ points. So, we first calculated the e-ph matrices using a $16 \times 16 \times 16$ $\mathbf{q}$ -point grid. Then, to check the convergence, we used a denser $32 \times 32 \times 32$ $\mathbf{q}$ -point mesh. For the additional $\mathbf{q}$ vectors, the matrix elements were calculated using a Fourier interpolation scheme for the change of the self-consistent potential with respect to atomic displacements as well as for the dynamical matrices. The maximum difference in $\lambda_{\mathbf{k}i}$ obtained for the two grids is 0.02. To assess the effect of local correlation on the electronic band structure, additional GGA + U calculations using an implementation within the mixed-basis pseudopotential approach [34] were performed.

III. RESULTS AND DISCUSSION

A. Structural parameters

ZrCo₂Sn belongs to the family of Heusler compounds which crystallize in the cubic $Fm\bar{3}m$ structure composed of four face-centered (fcc) sublattices mutually shifted by $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ along the body diagonal. The Zr and Sn atoms occupy fcc sublattices with the origins at (0,0,0) and $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, respectively. The Co atoms are located at $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ and $(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$ sublattices which are symmetry equivalent [see Fig. 1(a)].

The theoretical lattice parameter obtained by minimizing the total energy, $a = 6.304$ Å, is very close to the experimental value, $a = 6.254$ Å [20]. The deviation of $\sim 0.7\%$ is quite typical for calculations in the GGA-PBE approximation.

B. Band structure

Previous studies indicated that in combination with an approximation to the exchange-correlation functional, a Hubbard-like correction (+ U) should be employed for localized strongly correlated d electrons of Co (the value of $U = 3$ eV was used) to reproduce the Curie temperature close to the experimental value [13]. We therefore performed calculations for the electronic structure using both the GGA and the GGA + U . Both majority and minority bands of ZrCo₂Sn obtained within the GGA + U with $U = 3$ eV are shown in Fig. 1(c). As is known, the minority (spin-down) states in ZrCo₂Sn, as in many other Heusler compounds, are gapped around E_F [24]. This suggests that the electrons at the Fermi level are fully spin polarized and ZrCo₂Sn is a half-metallic ferromagnet [23]. The main effect of employing U is to increase the gap in the minority bands. However, the dispersion of majority bands in the spin-down gap remains unaffected, as can be seen in Fig. 1(d), which shows the majority bands calculated with $U = 0$. Therefore, the spin-up electronic states relevant for the present analysis of the EPC (in the energy range -0.2 eV $\leq E - E_F \leq 1.4$ eV) can be correctly calculated without taking the + U correction into account.

FIG. 1. (a) Crystal structure of ZrCo_2Sn : the $Fm\bar{3}m$ space group. (b) Phonon dispersion curves of ZrCo_2Sn calculated along the high-symmetry directions of the Brillouin zone. Lattice vibrations that make a decisive contribution to the scattering of electrons are indicated by dashed rectangles. (c, d) Calculated energy spectrum of ZrCo_2Sn . (c) Band structure obtained in the framework of GGA + U . Filled circles and dashed lines correspond to electronic bands with spin-up and spin-down, respectively. The Weyl point (indicated by W) is in the xy plane. The energy bands that form the Weyl point are denoted B1 and B2. The region where the electron-phonon interaction is analyzed is shown by dashed lines. (d) The majority bands calculated without + U are shown in accordance with the orbital localization of valence electrons: those mainly d_{z^2} , $d_{x^2-y^2}$ in character (Zr and Co) with an admixture of p Sn states are indicated by filled blue circles, and those purely d -like (Zr and Co d_{xz} , d_{yz} , d_{xy}) are shown by open circles. S1, S11, and S2 indicate the positions of electronic states for which a spectral representation of the e-ph coupling is presented.

When analyzing the e-ph interaction, we did not take into account the spin-orbit coupling (SOC) either. Since the strength of SOC in both Co and Zr is low, the SOC-induced modifications of the band dispersion around the Fermi level are insignificant and the half-metallic ferromagnetism of ZrCo_2Sn remains untouched in the relativistic calculations [13]. For example, our calculated density of majority states at the Fermi level, $N(E_F) = 0.855$ state/eV/atom, is in good agreement with the value obtained in the x-ray photoemission spectroscopy measurement, $N(E_F) = 0.86$ state/eV/atom [20].

Despite the weak influence on the dispersion of bands, the inclusion of the spin-orbit interaction is crucial for the Weyl physics because some symmetries can be broken when the two spin channels couple. In the absence of spin-orbit interaction, the band structure of ZrCo_2Sn features three topological nodal lines that become completely gapped after the introduction of SOC [13]. However, along the direction of magnetization ([110]), a pair of Weyl nodes survives. These Weyl points are 0.6 eV above the Fermi level in the ΓK symmetry direction and are protected by the C_{2110} rotation [13]. Therefore, in our

scalar relativistic calculation, we focus on the two electronic bands [B1 and B2 in Fig. 1(d)] that form the Weyl node in the ΓK direction. These majority bands are mainly d (Co and Zr) in character: one is a mixture of d_{z^2} , $d_{x^2-y^2}$ orbitals of Zr and Co with p Sn states, and the other is purely of d type (mainly d_{xz} , d_{yz} , d_{xy}). The energy position of the crossing point denoted by W in Fig. 1(d) is independent of whether or not the SOC is taken into account [13].

C. Phonon spectrum

Figure 1(b) shows the phonon dispersion of ZrCo_2Sn calculated with $U = 0$. We checked the effect of $U \neq 0$ on the phonon frequencies and dispersion by calculating some phonon modes with $U = 3$. The influence, on the whole, is very weak; the frequency changes are insignificant, of the order of hundredths of a meV, and they can be neglected.

Since the primitive unit cell of the cubic $Fm\bar{3}m$ structure consists of four atoms, there are 12 phonon branches. At the zone center the optical phonon modes correspond to the following irreducible representations: T_{2g} and $2T_{1u}$, which are all threefold degenerate. The T_{2g} mode generated by the

FIG. 2. (a, b) Electron-phonon coupling parameter λ_{ki} as a function of (a) the electron energy and (b) the momentum for the electronic bands B1 (filled blue circles) and B2 (open circles), which form the Weyl topological state in the ΓK symmetry direction. (c) Spectral decomposition of the e-ph coupling for electronic state S11 (solid line). The contribution of the B1 $\Rightarrow$ B2 transitions to $\lambda_{ki}(\omega)$ is shown by the shaded area. (d) The electron-phonon coupling parameter $\lambda(E)$ averaged over the electron momenta (filled circles) and the density of majority states $N(E)$ (open triangles) as a function of the energy. (e) Spectral decomposition of the e-ph coupling for electronic states, S1 (solid blue line) and S2 (dashed line). The position of the states is shown in Fig. 1(d). The shaded area shows $\lambda_{ki}(\omega)$ at an energy close to the crossing point (W).

opposing vibrations of Co atoms ($\sim 22 \text{ meV}$ at Γ) is Raman active. The remaining six T_{1u} modes (22.6 and 24.5 meV at Γ) are infrared active and are mainly determined by the opposing motion of Sn and Co atoms.

All the phonon modes have positive frequencies, which supports the dynamical stability of the compound. The mechanical stability of ZrCo_2Sn in the cubic $Fm\bar{3}m$ phase is also verified by the analysis of the calculated elastic constants: $C_{11} = 290.7 \text{ GPa}$, $C_{12} = 88.4 \text{ GPa}$, and $C_{44} = 129.6 \text{ GPa}$. We did not find any phonon anomaly in the phonon spectrum, unlike many other Heusler compounds, where acoustic modes tend to soften, and related anomalies were found in calculations of transverse acoustic branches along the $[110]$ direction [35,36]. Unfortunately, there are no experimental data on the phonon spectrum of ZrCo_2Sn for comparison.

D. Electron-phonon coupling

To see how the electronic states in the majority bands couple to phonons, we calculated the electron-phonon parameter λ_{ki} for the B1 and B2 electronic bands that form the Weyl node in the ΓK direction. Dotted lines in Fig. 1(c) mark

the region where the electron-phonon interaction is analyzed. The calculated λ_{ki} 's as a function of the electron energy and momentum are shown in Figs. 2(a) and 2(b). In general, the strength of the electron-phonon interaction in the region under consideration is moderate and varies between 0.1 and 0.3. As shown in the figure, the state-dependent e-ph coupling parameter shows a rather weak dependence on the hole (electron) energy and momentum position in the energy bands. In particular, in the energy interval from -0.2 to $+1.4 \text{ eV}$ with respect to E_F the variation range of λ_{ki} does not exceed 0.2.

Similar results were obtained for the momentum-averaged strength of the electron-phonon interaction, $\lambda(E)$, calculated at various energies around E_F ($-0.1 \text{ eV} \leq E \leq 1 \text{ eV}$). Figure 2(d) shows $\lambda(E)$ together with the density of majority electronic states, $N(E)$, at the same energy. The value averaged over all possible e-ph scattering events is centered around 0.35. At the crossing point (W), the strength of e-ph interaction is close to the minimum value: at an energy of 0.58 eV $\lambda_{ki} = 0.13$. Thus, the EPC in the topological Weyl state is weak enough to guarantee well-defined quasiparticles. However, when averaged over the momentum at this energy, it becomes more than twice as large, $\lambda(E) = 0.32$.

It is known that the coupling strength is largely determined by two factors: the number of final electronic states available for scattering processes with energies $\epsilon_{\mathbf{k}i} \pm \omega_{\mathbf{q}i}$ and the probability of scattering given by the EPC matrix elements. As shown in Fig. 2(d), in the energy range under consideration, the variation of $\lambda(E)$ is correlated with the available phase space. The same tendency was found in the topological surface states of Bi_2Se_3 and Bi_2Te_3 , where $\lambda_{\mathbf{k}i}$ shows monotonic growth with the electron energy, essentially following a linear increase in the density of states with the distance from the Dirac (crossing) point [9]. In the case of ZrCo_2Sn , the density of majority states in the spin-down energy gap varies around 0.3 state/eV, but the change in $\lambda_{\mathbf{k}i}$ with $N(E)$ is similar to that in the topological surface state of Bi_2Se_3 .

There are no restrictions on the phonon-induced scattering of electrons due to a peculiar spin texture of electronic states (for example, spin helicity), since all bands in the minority gap of ZrCo_2Sn are fully spin polarized, in contrast to the Dirac-like surface states in topological insulators.

The participation of various phonons in the electron scattering can be estimated from the spectral decomposition of the coupling constant, $\lambda_{\mathbf{k}i}(\omega)$, which gives the contribution of modes with a frequency ω to the total coupling strength. Figure 2(e) shows the spectral functions obtained for electronic states S1 and S2 with almost the same energy of ~ 0.95 eV in the B1 and B2 bands, respectively [see Fig. 1(c)]. Also shown is $\lambda_{\mathbf{k}i}(\omega)$ calculated at an energy close to the crossing point (W).

The dispersions shown in the figure are very similar, only the magnitude of some peaks increases with the distance from the crossing point, which reflects an increase in the e-ph coupling strength. In all spectra, the contributions of middle- and high-frequency lattice vibrations with $\omega \geq 12$ meV prevail, while low-energy (acoustic) phonon modes are weakly involved in the scattering of excited electrons and holes. This is a common feature for all considered electronic states. Analysis of the e-ph matrix elements also confirms that the probability of transitions with the participation of low-frequency phonons and, therefore, relatively small wave vectors is rather low.

In particular, this means that the probability of phonon-mediated transitions between the B1 and the B2 bands, especially near the crossing point, is low. At W, the strength of the e-ph coupling is determined by the scattering of electrons to other majority bands in the energy gap ($\sim 95\%$) and the rest is the Weyl part of the EPC due to transitions between two symmetry-related Weyl points. The contribution of transitions to electronic states in the immediate vicinity of the Weyl point, i.e., with a small transferred momentum, is negligible. Figure 2(c) shows the spectral function, $\lambda_{\mathbf{k}i}(\omega)$, calculated for the electronic state at an energy of 0.4 eV (band B1). The contribution of $\text{B1} \Rightarrow \text{B2}$ transitions (shaded area) to the e-ph scattering is less than 12%. Thus, for states with energies slightly different from W, the contribution of $\text{B1} \Rightarrow \text{B2}$ transitions to the phonon-induced scattering is still small, although it increases.

In general, the strength of the e-ph interaction in the B1 band is somewhat higher than in the B2 band at the same energy. So, at ~ 0.95 eV, the EPC strength in the S1 state (band B1) is about one and a half times larger than $\lambda_{\mathbf{k}i}$ for the S2

state (band B2). The band dependence of the e-ph interaction can be caused by slightly different orbital localizations of valence electrons in the crossing bands, as shown in Fig. 1(d). The e-ph coupling in the B2 band turns out to be weaker, since most of the electronic states available for scattering are of different orbital characters and the scattering in this case is less effective.

In the middle-energy part of the spectra, the contribution of short-wavelength lattice vibrations, indicated by dotted rectangles in Fig. 1(b), is important. Thus, a common feature of the spectral decomposition of $\lambda_{\mathbf{k}i}$ for both considered electron bands is a pronounced peak at 13–16 meV, which is mainly determined by the shear displacements of Co and Sn atoms. As for the zone-center optical vibrations, only those modes that are generated by mutually opposite vibrations of Co atoms actively participate in the e-ph interaction. These modes, with an energy of about 22 eV at the Γ point, belong to the threefold degenerate symmetry class T_{2g} and are Raman active. Interestingly, these phonons make a large contribution to e-ph scattering in YPd_2Sn , a superconducting Heusler compound with the same cubic structure, also only near the zone center [35].

IV. SUMMARY

The first-principles calculation shows that the electron-phonon coupling in the bands that form the topological Weyl state in the spin-down gap of ZrCo_2Sn has a moderate strength in the range from 0.1 to 0.3. When averaged over the electron momentum at a fixed energy the electron-phonon coupling constant $\lambda(E)$, which is essentially controlled by the available phase space, becomes somewhat larger, varying from 0.25 to 0.45. The e-ph coupling in electronic states close to the Weyl points is small enough to support well-defined quasiparticles. The EPC is also comparable to the e-ph scattering in the Dirac surface states of topological insulators.

The obtained state-dependent e-ph coupling parameter rather weakly depends on the electron (hole) energy and momentum. An analysis of the phonon modes carrying out the coupling shows that most of the modes actively involved in the scattering of excited electrons (holes) are middle- and high-frequency lattice vibrations. The probability of transitions mediated by small wave-vector phonons is rather low. The exception is those zone-center optical modes that are generated by mutually opposite vibrations of Co atoms, which is expected, since the spin-up electronic states located in the bandgap mainly consist of Co *d* electrons. The data obtained also indicate the dynamical stability of the compound and the absence of any phonon anomaly in the vibrational spectrum.

ACKNOWLEDGMENTS

This work was supported by the University of the Basque Country (Grants No. GIC07-IT-366-07 and No. IT- 756-13), the Spanish Ministry of Science and Innovation (Grant No. FIS2016-75862-P), and Saint Petersburg State University (ID 51126254). The authors acknowledge support by the state of Baden-Württemberg through bwHPC.

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