PAPER

Pressure-induced superconductivity in a shandite compound Pd$_3$Pb$_2$Se$_2$ with the Kagome lattice

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Abstract

High pressure electric transport and synchrotron x-ray diffraction (XRD) measurements together with the first-principles calculations are performed on a shandite compound Pd$_3$Pb$_2$Se$_2$ which contains the Kagome lattice of the transition metal Pd. A pressure-induced superconducting transition is observed above 25 GPa, for the first time in the shandite compounds, although the crystal structure of the compound seems to be very robust and persists up to the highest pressure in the XRD study (76.3 GPa). The superconducting transition temperature is about 2.2 K and almost does not change with pressure. The carrier density suddenly increases around 20 GPa possibly due to the emergence of two electron pockets at the $\Gamma$ point. Our work indicates that the superconductivity in Pd$_3$Pb$_2$Se$_2$ is strongly correlated to its electronic structure.

1. Introduction

The Kagome lattice is a two-dimensional network with corner-sharing triangles, which provided a fertile ground to study the frustrated, correlated and topological quantum electronic states [1–3]. The materials with such lattice structure have been extensively studied in geometrical spin frustration. Many novel physical phenomena such as quantum spin liquid, flat band and Dirac electronic states may emerge in this fascinating structure [4–10]. However, the materials with the Kagome lattice is relative rare.

The shandite compounds with the general formula $M_3A_2Ch_2$ ($M = \text{Co, Ni, Rh and Pd}; A = \text{Sn, Pb, In, Tl}; Ch = \text{S and Se}$) possess a rhombohedral-hexagonal structure with space group R$\overline{3}m$ (No. 166). The $M$ atoms form Kagome lattice stacking along c-axis direction. For the shandite compound, the half metal ferromagnetic Kagome-lattice Co$_3$Sn$_2$S$_2$ is recently suggested as a magnetic Weyl semimetal and shows a giant anomalous Hall conductivity [7, 8], which has attracted much attentions. However, few other shandite compounds have been investigated up to now.

Pressure is a clean method to directly tune the lattice parameters of materials which is crucial for both the magnetic properties and electronic structures. In addition, by applying high pressure, many topological materials can be tuned to superconductors [11–17]. However, the pressure effects of the shandite compounds are not well studied yet. Only Co$_3$Sn$_2$S$_2$ have been investigated under pressure as far as we known, the ferromagnetism in Co$_3$Sn$_2$S$_2$ is monotonically suppressed with increasing pressure and vanishes above 22 GPa [18]. For the other shandite materials, magnetism is absent, but no superconductivity was reported in these materials yet. By applying the pressure, the magnetic properties and electronic structures can be dramatically tuned, which may lead to the emergence of some novel physical properties in shandite compounds. Here, we focused on a shandite compound Pd$_3$Pb$_2$Se$_2$ which have been synthesized long time.
ago [19, 20], however, the details of its physical properties remain unknown. In this work, we successfully synthesized the high quality of Pd$_3$Pb$_2$Se$_2$ single crystal. By using the high-pressure x-ray diffraction (XRD) measurement, we find that its crystal structure remains the same up to 76.3 GPa. More intriguingly, superconductivity up to 2.2 K emerges at pressure above 25 GPa, and the $T_c$ is nearly unchanged with further increasing the pressure. By using the first-principles calculations, we find that the emergence of the superconductivity can be attributed to the change of the electronic structure, possibly related to the enhancement of the density of states (DOS) at high pressure. Our discovery of superconductivity in Pd$_3$Pb$_2$Se$_2$ indicates that intriguing physical properties can emerge in shandite materials besides the magnetic topological states.

2. Methods

Polycrystalline samples of Pd$_3$Pb$_2$Se$_2$ were synthesized by solid state reaction. The starting materials Pb lumps (purity 99.99%), Pd grains (purity 99.99%) and Se powers (purity 99.999%) were mixed together in stoichiometric and placed in an alumina crucible. Then, the crucible was sealed in an evacuated silica tube. The mixture was heated up to 1273 K with 50 K h$^{-1}$, then kept there for 48 h. Finally, the furnace was cooled down to room temperature after shutting down the power. Pd$_3$Pb$_2$Se$_2$ single crystals were grown by heating the Pd$_3$Pb$_2$Se$_2$ polycrystalline to 1223 K under 1.5 GPa in a cubic-anvil-type apparatus (Riken CAP-07), keeping the temperature for 1 h, and then slowly cooled to 963 K with a cooling rate of 26 K h$^{-1}$.

The basic magnetism of the Pd$_3$Pb$_2$Se$_2$ single crystals were measured in SQUID magnetometer (MPMS-5 T, Quantum Design). Diamond anvils with 200 μm culet and c-BN gasket with 70 μm sample chambers were used for transport measurements. NaCl was used as a pressure transmitting medium and the pressure was calibrated by using the shift of ruby florescence at room temperature [21]. During transport measurements, the pressure was applied at room temperature using the miniature diamond anvil cell [22]. The resistance and Hall coefficient were measured using the Quantum Design PPMS-9 with alternating current. We used the van der Pauw method to measure the resistance and Hall coefficient under pressure. The low temperature ($<$ 2 K) measurements were conducted in a dilution refrigerator (Kelvinox JT, Oxford Instruments). The temperature sensor was mounted on the cell. The high-pressure synchrotron XRD was carried out at room temperature at the beamline BL15U1 of the Shanghai synchrotron radiation facility (SSRF) with wavelength $\lambda = 0.6199$ Å. A symmetric diamond anvil cell with a pair of 300 μm culet size anvils was used to generate pressure and Daphne 7373 oil was loaded as pressure transmitting medium. GSAS was used to refine the data using the Le Bail method [23].

The crystal structure optimizing and self-consistent total energy calculations were performed with VASP [24] utilizing the GGA approximation with the PBE exchange-correlation functionals [25]. An energy cutoff for plane-wave basis cutoff of 375 eV and a $\Gamma$-centered k-points mesh with spacing of $2\pi \times 0.02$ Å$^{-1}$ were employed. The band structures were checked with Tran–Blaha modified Becke–Johnson xc-potential [26]. Due to the presence of the heavy elements, the electronic structure, including band structures, DOS and Fermi surfaces, were calculated with the consideration of spin orbital coupling (SOC) effect. Phonon spectra were calculated with the PHONOPY package [27].

3. Results and discussion

The crystal structure of Pd$_3$Pb$_2$Se$_2$ is presented in figure 1(a). Superconductivity up to 13 K was observed in pressurized PbSe$_2$ with pyrite structure [28], however, the structure between these two materials are quite different. Pd$_3$Pb$_2$Se$_2$ is composed of the slabs of PdPb$_4$Se$_2$ octahedra stacking with a hexagonal packing along the c-axis direction. Each Pd atom is coordinated with four Pb atoms and two Se atoms, forming a distorted octahedron. The Pd atoms form perfect Kagome lattice in Pd–Pb layer as shown in the right side of figure 1(a). There are two kinds of Pb sites. A half of Pb atoms (orange spheres) connecting adjacent Pd–Pb layers, and another half of Pb atoms (red spheres) locate in the centers of the Kagome hexagons in Pd–Pb layer. Figure 1(b) displays the XRD pattern of a Pd$_3$Pb$_2$Se$_2$ single crystal. Only (00l) diffraction peaks can be detected, indicating the pure phase of the as-grown single crystal with a [001] preferred orientation direction. The c-axis lattice parameter can be determined to be 14.601 Å, which is consistent with the previous reported value of Pd$_3$Pb$_2$Se$_2$ [20]. The temperature dependence of resistivity at ambient pressure is presented in figure 1(c), which shows metallic behavior at full temperature range. At the room temperature, the resistivity is 0.13 mΩ cm and decreases to 0.031 mΩ cm at $T = 2$ K, yielding a residual-resistivity-ratio of 4.2. Figure 1(d) shows the temperature dependence of the magnetic susceptibility $\chi(T)$ with a magnetic field of 10 kOe applied along c-axis direction. The susceptibility is small and shows a broad hump around 50 K, which indicate the main contribution of the susceptibility is from
Figure 1. (a) Crystal structure of Pd₃Pb₂Se₂ and Kagome lattice made of Pd atoms. The blue and green spheres represent Pd and Se atoms, respectively, and the brown and red spheres represent Pb atoms at Pb₁ and Pb₂ sites, respectively. (b) XRD pattern of Pd₃Pb₂Se₂ single crystal with the corresponding Miller indices (00L) in parentheses. (c) Temperature dependence of the resistivity at ambient pressure. (d) Temperature dependence of magnetic susceptibility $\chi(T)$ measured with applied magnetic field $H = 10$ kOe along c-axis direction.

the Pauli paramagnetism. No phase transitions can be detected from the resistivity and susceptibility measurements performed at ambient pressure.

In order to seek for novel quantum states in Pd₃Pb₂Se₂, we applied high pressure to directly tune its electronic structure. We first performed the high-pressure electrical transport measurement with pressure up to nearly 80 GPa as shown in figure 2. Pd₃Pb₂Se₂ shows typical metallic behavior, which is characterized by monotonic increasing of resistance with increasing temperature, and exhibits a lower room-temperature resistance with increasing the pressure up to 19.6 GPa as shown in figure 2(a). The trend is reversed above 26.5 GPa as shown in figure 2(b), the resistance starts to increase with further increasing the pressure. More intriguingly, the resistance suddenly decreases below 2.2 K with pressure above 26.5 GPa which is possibly due to a superconducting transition. The inset of figure 2(b) shows the normalized resistance at the low-temperature region. The onset of the transition temperature is nearly invariant with the pressure. As the pressure continues to increase, the resistance drops more sharply, but does not reach zero even at 1.85 K.

To further support that the resistance drops observed in pressurized Pd₃Pb₂Se₂ is related to a superconducting transition, we performed high-pressure transport measurements in a dilution refrigerator with lowest temperature $\sim 0.1$ K. As shown in figure 3(a), zero resistance is observed at 37.8 and 77.5 GPa, which is the direct evidence of superconducting transition. We can also apply magnetic field to suppress the superconducting transition. Figures 3(b) and (c) show the suppression of superconductivity under various magnetic fields with pressure at 37.8 and 77.5 GPa, respectively. It is obvious that $T_C$ shifts toward lower temperature with increasing the magnetic field, indicating the transition is due to superconductivity in nature. Figure 3(d) shows the temperature dependence of the upper critical field $H_{C2}$ for the pressure at 37.8 and 77.5 GPa. The $T_C$ is determined by using 90% normal state resistance criterion. The $H_{C2}$ at zero temperature can be estimated to be 0.75 and 1.25 T for the pressure at 37.8 and 77.5 GPa, respectively. Although the $T_C$ is nearly invariant under pressure, the $H_{C2}$ at higher pressure is much larger than that at lower pressure. In order to approximate the superconducting parameters, we have used the Ginzburg–Landau formula to calculate the coherence length $\xi$, $\xi = (\Phi_0 / 2\pi \mu_0 H_{C2})^{1/2}$, where $\Phi_0 = 2.07 \times 10^{-7}$ Oe cm², the coherence length $\xi$ at zero temperature can be estimated to be 21 and 16 nm for the pressure at 37.8 and 77.5 GPa, respectively.

It is of great interest to clarify the Hall resistance before and after the superconducting transition because these quantities can reflect the effect of pressure on the electronic structure. Building on these ideas, we performed high-pressure Hall resistance measurements on the Pd₃Pb₂Se₂ single crystal by sweeping the
Figure 2. Temperature dependences of electrical resistance for Pd₃Pb₂Se₂ single crystal under various pressures. (a) Temperature-dependent resistance measured from 1.0 to 19.6 GPa. The resistance gradually decreases with increasing the pressure. (b) Temperature-dependent resistance measured with the pressures between 26.5 to 77.5 GPa. The superconducting transition emerges below 2.2 K. The inset shows the normalized resistance around the superconducting transition region.

Figure 3. (a) The temperature-dependent resistance around superconducting transition temperature measured in the dilution refrigerator with the pressure at 37.8 GPa (red circle line) and 77.5 Ga (blue triangle line). (b) and (c) Temperature dependence of resistance measured under various magnetic fields at 37.8 GPa and 77.5 Ga. (d) The derived upper critical field $H_{c2}$ as a function of superconducting transition temperature $T_c$ at 37.8 GPa (red circle line) and 77.5 GPa (blue triangle line).

magnetic field up to 4 T at 10 K at various pressures as shown in figure 4(a). The Hall resistance evolves linearly with magnetic field and shows negative slopes at 10 K for all the pressures, implying that electron-type carriers are dominant in Pd₃Pb₂Se₂. We can derive the Hall coefficient ($R_H$) and carrier concentration ($n$) under various pressures as shown in figure 4(b). Upon compression, $n$ increases and $R_H$ decreases with increasing pressure. The carrier density exhibits a sudden increment around 20 GPa which is possibly due to the pressure-induced electronic phase transition.
In order to investigate the structural evolution at high pressure, we performed the high-pressure XRD measurements on the Pd$_3$Pb$_2$Se$_2$ sample up to 76.3 GPa as shown in figure 5. The XRD patterns collected at different pressures are displayed in figure 5(a). It is found that all the observed peaks can be well indexed by using its ambient pressure structure (selected Le Bail fits of the XRD patterns can be found in the supplemental materials (https://stacks.iop.org/NJP/22/123013/mmedia)), which indicates that the structure of Pd$_3$Pb$_2$Se$_2$ remains stable with pressure up to 76.3 GPa. Since the resistance evolves smoothly with the temperature above $T_C$, the sample is unlikely to have a structural phase transition at low temperature. The derived lattice parameters $a$ and $c$ as a function of pressure are shown in figure 5(b). The inset of figure 5(b) shows $c/a$ as a function of pressure. $c/a$ slightly increases with increasing the pressure, with the pressure above 30 GPa, it becomes almost a constant. The slightly increment of $c/a$ ratio with increasing the pressure is similar to an isostructural material Co$_3$Sn$_2$S$_2$ [18], because the structure of shandite materials is
Figure 6. (a)–(h) Band structures of Pd$_3$Pb$_2$Se$_2$ with SOC effect at 0, 10.3, 16.6, 20, 25.2, 30, 40.8 and 60 GPa, respectively. Green lines represent the bands that already cross the Fermi level at 0 GPa and the cyan lines represent the bands that move to Fermi level at high pressure. The black circle indicates the vHS.

Figure 7. (a)–(f) DOS of Pd$_3$Pb$_2$Se$_2$ with SOC effect at 0, 16.6, 25.2, 30, 40.8 and 60 GPa, respectively. A vHS around Fermi energy appears above 25 GPa.

three-dimensional with strong interlayer bonding. The derived cell volume is shown in figure 5(c), which can be well fitted by using the Birch–Murnaghan equation of state with the derived bulk modulus $B_0 = 62.1$ GPa.

In order to clarify the electronic structure and origin of superconductivity, we performed the first-principles calculations at high pressure. The calculated electronic band structures for Pd$_3$Pb$_2$Se$_2$ are shown in figure 6. By applying the pressure, two electron bands moved down and across the Fermi level at about 16.6 GPa, which is consistent with the Hall measurement. Further increasing the pressure, one of the electron bands starts to move up and above the Fermi level with the pressure about 40.8 GPa. We also calculate the DOS under pressures as shown in figure 7. The DOS at ambient pressure is relatively low, by increasing the pressure, the DOS increases gradually. When it comes to the pressure at which superconductivity emerges (about 25 GPa), a sharp peak around the Fermi energy appears. This sharp peak in the DOS is related to the van Hove singularity (vHS), which is related to the minimum points along $\Gamma$–$Z$, $\Gamma$–$L$ directions of the electronic structure in figure 6, marked with black circles. Because vHS near the Fermi level will usually increase the electron density and may enhance the electron–phonon coupling [29], which are beneficial for the superconductivity. Thus, we conjectured that higher DOS from the tail of the vHS may be an important reason for the superconductivity, however may be not the exclusive factor, just as discussed in the other vHS systems [29–32]. Although the vHS slightly shift away from the Fermi level at
higher pressure which would lead to the reduction of DOS, the Debye temperature may slightly increase with increasing the pressure [33, 34] and this may explain the phenomenon observed in experiment that the superconducting transition temperature almost does not change with pressure. The reduction of the resistance below 20 GPa can be attributed to the enhancement of carrier density, which is possibly related to the two electron pockets across the Fermi level at the $\Gamma$ point. The increment of the resistance above $\sim 27$ GPa can be attributed to the reduction of the mobility at high pressure. We also show the Fermi surface of Pd$_3$Pb$_2$Se$_2$ at various pressures to illustrate the changes of band structures as shown in figure 8. The Fermi surface changes dramatically below 16.6 GPa, consistent with Hall coefficient measurement. There are five Fermi surfaces when pressure reach to 16.6 GPa, and the first two Fermi surfaces are rather complex and the later three are ball-like. The sudden emergent of the latter two Fermi pockets result in the sharp increase of the carrier density at 16.6 GPa.

Although a bunch of shandite compounds had been synthesized before, superconductivity was never reported in this type of materials. As far as we known, our discovery of the superconductivity up to 2.2 K in Pd$_3$Pb$_2$Se$_2$ is the first case. The Kagome structure of the $M$ ions makes this type of material intriguing due to its relation to the widely discussed Kagome-lattice models. For instance, the magnetic Kagome-lattice materials such as Co$_3$Sn$_2$S$_2$, Fe$_3$Sn$_2$, Mn$_3$Sn exhibit large anomalous Hall resistivity due to the contribution of Berry curvature [5–9]. Thus, introducing the magnetism in the shandite compounds would be interesting. For Pd$_3$Pb$_2$Se$_2$, we cannot detect any magnetic phase transitions in the $R$–$T$ curve, however, the spin fluctuation due to the Kagome lattice may exist at high pressure which needs further investigation.

4. Conclusion

In conclusion, we systematically investigate the pressure effect of a shandite compound Pd$_3$Pb$_2$Se$_2$ which contains the Kagome lattice of the transition metal Pd. No structural phase transition is observed up to 76.3 GPa. The carrier density gradually increases with increasing the pressure and shows an anomaly around 20 GPa, which is probably due to the emergence of two electron pockets at the $\Gamma$ point. The superconductivity emerges above 25.6 GPa, and the $T_C$ ($\sim 2.2$ K) is almost invariant with the pressure. The origin of the superconductivity is related to the change of the electronic structure, possibly due to the emergence of a vHS around Fermi level.

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