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Structural and Transport Properties of the Weyl Semimetal NbAs at High Pressure *

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We perform a series of high-pressure synchrotron x-ray diffraction (XRD) and resistance measurements on the Weyl semimetal NbAs. The crystal structure remains stable up to 26 GPa according to the powder XRD data. The resistance of NbAs single crystal increases monotonically with pressure at low temperature. Up to 20 GPa, no superconducting transition is observed down to 0.3 K. These results show that the Weyl semimetal phase is robust in NbAs, and applying pressure may not be a good way to obtain a topological superconductor from Weyl semimetal NbAs.

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Following the intensive studies of topological insulators (TIs),[1] recently a great deal of interest has been shown in three-dimensional (3D) topological semimetals,[2–11] in which the conduction and valence bands touch at isolated points in the Brillouin zone, and the electrons have relativistic dispersion. Weyl semimetal (WSM) is one type of such materials, and it is characterized by the Weyl nodes, which always exist in pairs with opposite chirality.[7,8] To obtain WSM, either time reversal or inversion symmetry needs to be broken.[5,6] Though it is theoretically predicted to occur in strongly spin-orbit coupled systems, the existence of 3D WSMs are very rare in nature.[2,3] The topologically nontrivial 3D Dirac semimetal (DSM) is proposed to be protected by the proper crystal symmetry when band inversion and time-reversal symmetry are present.[5,6] Such protected Dirac nodes are four-fold degenerate states including spin degeneracy. In 3D DSMs, the degenerate Dirac point is composed of two overlapping Weyl points with opposite chirality.[9]

The 3D DSM phase has been experimentally discovered in Na_3Bi and Cd_3As_2,[12–18] after the theoretical predictions.[5,6] More recently, a family of noncentrosymmetric 3D WSM, the stoichiometric TaAs, TaP, NbAs and NbP with no inversion center in the crystal structure, was predicted.[10,11] A series of experiments have been performed on this family to search for the proposed WSM state.[19–26] As hallmarks of the WSM state, both the Fermi arcs on the (001) surface and Weyl nodes in the bulk have been observed in TaAs and NbAs from ARPES measurements.[19–22] Extremely large magnetoresistance and ultra-high mobility were reported from transport measurements in TaAs, NbAs and NbP.[23–26] Furthermore, negative magnetoresistance due to the chiral anomaly of Weyl fermions was also observed in TaAs.[26]

Starting from the topological semimetals, one may expect to obtain topological superconductors (TSCs) by carrier doping or applying pressure.[6,27] The TSCs have a full pairing gap in the bulk and gapless surface states consisting of Majorana fermions.[1] Previously, a few candidates of TSC have been found by doping or pressurizing TIs.[28–37] For 3D DSM Cd_3As_2, superconductivity has been reported under high pressure, after a structural phase transition.[38] The realization of pressure-induced superconductivity in these topological materials motivated us to study the high-pressure effects on WSMs. To the best of our knowledge, there has been no pressure study on the above-mentioned WSMs (TaAs, NbAs and NbP). It will be very interesting to investigate whether pressure can induce superconductivity in them.

In this Letter, we report the high-pressure powder x-ray diffraction and single crystal resistance measurements on the WSM NbAs. It is found that the crystal structure remains unchanged, and only the lattice parameters decrease slightly with the increasing pressure. From the resistance measurements, no supercon-

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ducting transition is observed down to 0.3 K and up to 20 GPa. These results show the robustness of the WSM phase in NbAs, and suggest that pressurizing a WSM may be not a good way to obtain a topological superconductor.

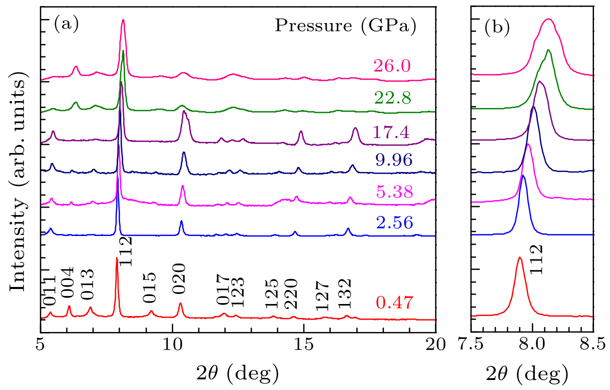

Fig. 1. In-situ powder synchrotron XRD patterns of NbAs under various pressures up to 26 GPa at room temperature, with the x-ray wavelength $\lambda = 0.3100$ Å. (b) Pressure evolution of the (112) peak. The shift towards higher angle indicates the shrink of the lattice under pressure.

The NbAs single crystals were grown using the Sn flux method.[39] After getting rid of the Sn flux, shinning single crystals with typical dimensions of $100 \times 100 \times 80\,\mu m^3$ were obtained. They are very stable in air and water. By using a Mao–Bell type diamond anvil cell (DAC),[40] the *in situ* powder synchrotron XRD experiments were carried out at the High-Pressure Collaborative Access Team (HPCAT), at the Advanced Photon Source of Argonne National Laboratory. The powder was prepared by grinding several pieces of single crystals. For resistance measurements, the thickness of NbAs single crystals was reduced to ∼20 µm by mechanically polishing. Four Pt electrodes were attached to the sample corners with silver epoxy. Resistance measurement under ambient pressure was performed in a physical property measurement system (PPMS, quantum design). For high-pressure resistance measurements, the sample was loaded into the chamber together with ruby powder for pressure determining. The silicon oil was used as the pressure-transmitting medium. The high-pressure resistance measurements were performed in an ^{3}He cryostat, by the van der Pauw method. All the samples used in this work were from the same batch.

We first performed the high-pressure powder XRD measurements to examine the structural stability of NbAs. NbAs crystallizes in a body-centered tetragonal Bravais lattice with the noncentrosymmetric tetragonal space group of $I4_1md$ (#109). There is a single site for both Nb and As atoms in the unit cell and the atomic coordinates of Nb and As are $(0, 0, 0)$ and $(0, 0, 0.416)$, respectively.[41,42] Figure 1(a) displays the XRD patterns of NbAs under various pressures at room temperature. Under low pressure $p =$ 0.47 GPa, all the peaks can be indexed with space group $I4_1md$, and the lattice parameters $a = 3.453$ Å and $c = 11.677$ Å are obtained by fitting the XRD data with GSAS software. These values agree well with the previous reports under ambient pressure.[41,42] With the increasing pressure, one can see that the overall XRD pattern does not change. The major (112) peak only shows a slight shift towards a higher angle, as plotted in Fig. 1(b). This shift indicates the shrink of the lattice under pressure. Under the highest pressure $p = 26$ GPa we applied in this study, the lattice parameters decreased by 3–4%, to $a = 3.366$ Å and $c = 11.206$ Å. These results show that the crystal structure of WSM NbAs is very stable under pressure.

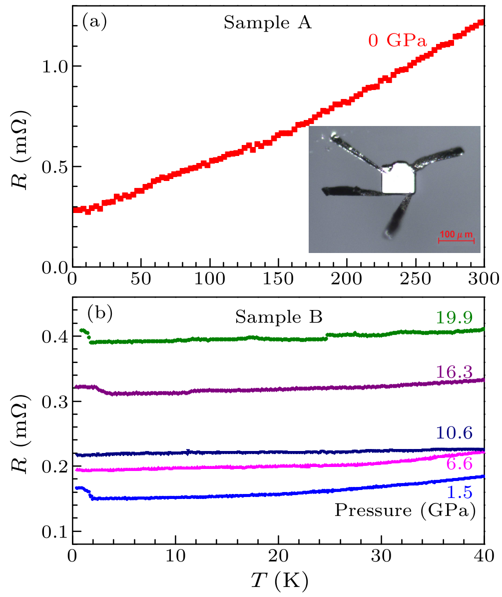

Fig. 2. The resistance of NbAs single crystal under various pressures. (a) The value of $R(T)$ of sample A measured at ambient pressure. (b) The value of $R(T)$ of sample B measured under pressures up to 20 GPa. Inset: the typical configuration of resistance measurement for NbAs single crystal. Four Pt electrodes were attached to the sample corners with silver epoxy.

Figure 2(a) shows the temperature dependence of resistance $R(T)$ for NbAs single crystal (sample A) measured at ambient pressure. The resistance decreases with temperature down to 2 K, with the residual resistance ratio RRR$=R(300\,\mathrm{K})/R(2\,\mathrm{K})\approx 6$. This metallic behavior is consistent with that of the previously reported polycrystalline sample (RRR≈2).[42] In Fig. 2(b), the low-temperature resistance of sample B under various pressures up to 20 GPa are plotted. With the increasing pressure, $R(T)$ remains metallic, while its absolute value increases monotonically. At the very low temperature, there is a small resistance upturn under several pressures ($p = 1.5$, 16.3, and 19.9 GPa), the origin of which is unclear. Nevertheless, no superconducting transition is observed down to 0.3 K under pressure up to 20 GPa. The slight change of $R(T)$ and the absence of superconductivity demonstrate that the WSM state in NbAs is very robust under pressure.

Therefore, no dramatic pressure effects are observed on both crystal structure and electronic state of WSM NbAs. This situation is quite different from that of 3D TIs and DSM Cd_3As_2.[32−38,43] For example, TI Bi_2Se_3 shows a structural phase transition from rhombohedral (R-$3m$) to monoclinic ($C2/m$) structure near 10 GPa, and the pressure-induced superconductivity was observed above 13 GPa.[36] Structural phase transition and superconductivity were also reported in three other TIs (Bi_2Te_3, Sb_2Se_3, and Sb_2Te_3) under pressure.[32−35,37] For the 3D DSM Cd_3As_2, it undergoes a structural phase transition from tetragonal ($I4_1/acd$) to monoclinic ($P2_1/c$) structure near 3 GPa,[43] and pressure-induced superconductivity was reported above 8 GPa.[38] All these structural phase transitions occur from a high-symmetry space group to a low-symmetry one. The crystal structure of NbAs does not change under pressure possibly due to the fact that it is already in a low-symmetry space group. In this context, the robustness of the WSM state in NbAs may relate to its stable crystal structure.

In summary, we have investigated the pressure effects on the crystal structure and electronic state of the WSM NbAs. The powder XRD results show that the crystal structure is stable up to 26 GPa. No resistive superconducting transition is observed down to 0.3 K under pressure up to 20 GPa. It is concluded that the Weyl semimetal state is robust in NbAs, and applying pressure may not be a good way to obtain a topological superconductor from Weyl semimetal NbAs.

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