Observation of Negative Magnetoresistance and nontrivial $\pi$ Berrys phase in 3D Weyl semi-metal NbAs

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We report the electric transport properties of NbAs, which is a Weyl semimetal candidate proposed by recent theoretical calculations and confirmed by recent angle-resolved photoemission spectroscopy (ARPES) data. We detected the long-anticipated negative magneto-resistance generated by the chiral anomaly in NbAs. Clear Shubnikov de Haas (SdH) oscillations have been detected starting from very weak magnetic field. Analysis of the SdH peaks gives the Berry phase accumulated along the cyclotron orbits to be $\pi$, indicating the existence of Weyl points.

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Predicted to show unprecedented features beyond the classical electronic theories of metals, Weyl semi-metal (WSM) has motivated much interest for the realization of electronic topological properties. The appearance of Weyl points near the Fermi level will cause novel electronic properties and usually not very sensitive to the magnetic field. The proposal have stimulated enormous interests. The existence of Weyl nodes has soon been discovered in TaAs by angle-resolved photoemission spectroscopy (ARPES) data. We detected the long-anticipated negative magnetoresistance generated by the chiral anomaly in NbAs. Clear Shubnikov de Haas (SdH) oscillations have been detected starting from very weak magnetic field. Analysis of the SdH peaks gives the Berry phase accumulated along the cyclotron orbits to be $\pi$, indicating the existence of Weyl points.

Niobium arsenide, NbAs, crystallizes in a body-centered tetragonal Bravais lattice, space group I41md (109). Our X-ray diffraction (XRD) obtains lattice constants of $a = 3.45$ Å and $c = 11.68$ Å, consistent with the earlier crystallographic studies. Single crystals of NbAs were grown by vapor transport using iodine as the transport agent, as described in Ref. 24. First, polycrystalline NbAs was prepared by heating stoichiometric amounts of Nb and As in an evacuated silica ampoule at 973 K for 1 day. Subsequently, the powder was loaded in a horizontal tube furnace in which the temperature of the hot zone was kept at 1223 K and that of the cold zone was at 1123 K. The crystals of NbAs were verified by powder x-ray diffraction (XRD) and by compositional analysis conducted using an energy dispersive x-ray spectroscopy (EDS). An atomic percentage ratio of Nb:As = 49.4 : 50.6 was obtained on the EDS measurements. The largest natural surface of the obtained NbAs single crystals was determined to be the (112) plane by single crystal x-ray diffraction, shown in the lower inset of Fig. 1(a), with typical dimension of $1 \times 1$ mm$^2$. The quality of the NbAs single crystals was further checked by the x-ray rocking curve. The full width at half maximum (FWHM) is only $0.03^\circ$ (not showing here), indicating the high quality of the single crystals. The sample was polished to a bar shape, with $1 \times 0.3$ mm$^2$ in the (112) plane and a 0.2 mm thickness. A standard six-probe method was used for both the longitudinal resistivity and transverse Hall resistance measurements.

Recently, using first principle calculations, Weng et al. predicted that non-centrosymmetric TaAs, TaP, NbAs and NbP, are time-reversal invariant 3D WSMs with a dozen pairs of Weyl nodes which are generated by the absence of inversion center. The proposal have stimulated enormous interests. The existence of Weyl nodes has soon been discovered in TaAs by angle-resolved photoemission spectroscopy (ARPES) data. We detected the long-anticipated negative magneto-resistance generated by the chiral anomaly in NbAs. Clear Shubnikov de Haas (SdH) oscillations have been detected starting from very weak magnetic field. Analysis of the SdH peaks gives the Berry phase accumulated along the cyclotron orbits to be $\pi$, indicating the existence of Weyl points.
emphasizing the contrast between extremely large positive MR for magnetic field perpendicular to current ($\theta = 90^\circ$) and negative MR for field parallel to current ($\theta = 0^\circ$). The right inset of Fig. 1(a) depicts the corresponding measurement configurations. Fig. 1(b) presents the MR at various temperatures, when magnetic field parallel to the current ($\mu_0 H//I$, $\theta = 0^\circ$). And the inset of Fig. 1(b) display the original resistivity data. Below 20 K, an negative MR of about -20% can be observed under an applied field of 3.2 T. Then, the negative MR is suppressed with increasing temperature, and ultimately disappeared at higher temperature, similar with the result in ZrTe$_5$ and TaAs. The existence of chiral quasi-particles in Dirac and Weyl semimetals opens the possibility to observe the effects of the chiral anomaly. The chiral magnetic effect, which is the generation of electric current in an external magnetic field induced by the chirality imbalance, is of particular interest. The most prominent signature of the chiral magnetic effect in Dirac systems in parallel electric and magnetic fields is the positive contribution to the conductivity that has a quadratic dependence on magnetic field. The chiral anomaly contributed conductivity as $\sigma = (e^2 v_F^2 / 4 \pi^2 h^2 c^2) B^2$ where $\tau$ is the inter valley scattering time, $v_F$ is the Fermi velocity near the Weyl points and $\mu$ denotes the chemical potential measured from the energy of the Weyl points. This is because the chiral magnetic effect current is proportional to the product of chirality imbalance and the magnetic field, and the chirality imbalance in Dirac systems is generated dynamically through the anomaly with a rate that is proportional to the product of electric and magnetic fields $E \cdot B$. As a result, the longitudinal MR becomes negative, which has the maximum effect with $E$ parallel to $B$. Of course the total conductivity of the system will also include other contributions from the non-chiral states as well, which may weaken the negative MR effect or even overwhelm it if the non-chiral part dominates the DC transport, which may be the case in ref. The phenomena may due to the Coulomb interaction among the electrons occupying the chiral states. Since the degeneracy of the chiral states as well as the density of states at the Fermi level goes linearly with the magnetic field, eventually the system will approach a spin-density-wave (SDW) like instability under Coulomb interaction. Then at finite temperature, the strong SDW fluctuation provides an-

Figure 1(a) displays the field dependence of MR measured at $T = 2$ K for several angles $\theta$ of the applied magnetic field ($\mu_0 H$) with respect to the electric current ($I$). The angle rotates from $\mu_0 H//I$ to $\mu_0 H\perp I$, so that at $\theta = 0^\circ$, the applied field is parallel to the current ($\mu_0 H//I$), which is the so-called Lorentz force free configuration. When the magnetic field is applied perpendicular to the current ($\mu_0 H\perp I$, $\theta = 90^\circ$), a positive MR of up to 10000% is observed. This large transverse MR strongly relies on $\theta$. When the magnetic field is rotated to be parallel to the electric current ($\theta = 0^\circ$), we get a negative MR, which is an indication of chiral magnetic field and should be a strong evidence of Weyl fermions in NbAs. The left inset of Fig. 1(a) displays the original resistivity data plotted on logarithmic scale,
other scattering channel which can be greatly enhanced in high field and may give the positive MR in the high field region\textsuperscript{16}.

Figure 2(a) displays the magnetic field dependence of Hall resistivity $\rho_{yx}(B//c)$ measured at various temperatures. At low temperature, the negative slope in high magnetic fields indicates that the electrons dominate the main transport processes. However, in low fields the curve tends to be flat. At 100 K and 150 K, for example, $\rho_{yx}$ is initially positive under low fields but changes to negative in higher fields. The curvature and sign reversal of the Hall resistivity indicates the coexistence of hole-type minority carriers with high mobility and electron-type majority carriers with low mobility. At higher temperature slope of Hall resistivity changes to positive, implying the carriers dominating the conduction mechanism transformed to hole-type. All these are consistent with multiple hole- and electron-like carriers as was also observed in TaAs and NbP, and indicated by band structure calculations\textsuperscript{16,21,34,35} and a previous paper on NbAs\textsuperscript{24}.

As shown in Fig. 2(b), the material show negative Hall coefficient, $R_H(T)$, up to 150 K and then changes sign for temperature above about 150 K. For the sake of simplicity, we use the single band to estimate the mobility. The inset of Fig 2(b) displays mobility versus temperature determined by the Hall coefficient at 7 T and the zero field resistivity using a single band approximation. The mobility plays a major role for charge transport in a material, and consequently decides the efficiency of various devices. Here, NbAs exhibits an ultrahigh mobility of $2.45 \times 10^5$ cm$^2$/Vs at 1.5 K, consistent with the result in ref.\textsuperscript{24}.

In Fig. 3(a) the temperature dependence of resistivity is plotted. The inset gives the measurement configuration. In zero magnetic field, NbAs exhibits a metallic behavior down to 1.5 K. The applied magnetic field not only significantly increases the resistivity, but also stimulates a crossover from metallic to insulator like behavior, which may be related to the formation of the Landau levels under magnetic field\textsuperscript{10}. Under applied field, a resistivity anomaly can be observed, which can be enhanced
from very weak magnetic field. de Haas (SdH) oscillations have been detected starting with the frequency of 25 T. The cross-sectional area of the data points in Fig. 4 can be fitted linearly, and the linear extrapolation gives an intercept 0.119, which means a non-trivial π Berry’s phase (β = 1/2) and δ = 0.119 (very close to 1/8), signaling the 3D Dirac fermion behaviors, and implying the FS associated with 25 T quantum oscillations is enclosing a Weyl point.

In the trivial parabolic dispersion case such as that involving conventional metals, the Berry’s phase 2πβ should be zero. For Dirac systems with linear dispersion, there should be a nontrivial π Berry’s phase (β = 1/2). This non-trivial π Berry’s phase has been clearly observed in 2D graphene, bulk Rashba Semiconductor BiTeI, bulk SrMnBi2 in which highly anisotropic Dirac fermions reside in the 2D Bi square net, 3D Dirac Fermions Cd3As2, and recently in Weyl semi-metal TaAs. The intercept 0.119 obtained in Fig. 4 clearly reveals the nontrivial π Berry’s phase, and thus provides strong evidence for the existence of Weyl fermions in NbAs. An additional phase shift δ = 0.119 ~ 1/8 should result from the 3D nature of the system. Complementary to previous theoretical and ARPES experiments results, our bulk transport measurements confirm the 3D Dirac semimetal phase in NbAs.

In summary, we have performed bulk transport measurements on single crystals of the proposed 3D Weyl semimetal NbAs. Large MR as high as 10000% is detected with magnetic field perpendicular to the current. When the external magnetic field is rotated to be parallel with the current, Chiral anomaly induced negative MR up to -20% is observed. This unusual negative MR is the first electric transport evidence for the chiral anomaly associated with the Weyl points in NbAs. Hall effect data suggest that both n and p types of carriers exist in NbAs. NbAs exhibits an ultrahigh mobility of 2.45 × 10^5 cm²/Vs at 1.5 K. A large linear quantum magnetoresistance is observed at room temperature. By analyzing the Shubnikov de Haas oscillations of longitudinal resistance at low temperature, a nontrivial π Berry’s phase with a phase shift of 0.119 is obtained, which provides bulk quantum transport evidence for the existence of a 3D Weyl semimetal phase in NbAs. With its unique electronic structure, unusual high mobility, and large room-temperature linear magnetoresistance, the 3D Weyl semimetal NbAs may open new avenues for future device applications.

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