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Anisotropic resistivity and Hall effect in MgB_2 single crystals

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We report resistivity and the Hall-effect measurements in the normal and superconducting states of MgB_2 single crystals. The resistivity has been found to be anisotropic with slightly temperature-dependent resistivity ratio of about 3.5. The Hall constant, with a magnetic field parallel to the Mg and B sheets, is negative in contrast to the holelike Hall response with a field directed along the c axis, indicating presence of both types of charge carriers and, thus, the multiband electronic structure of MgB_2. The Hall effect in the mixed state shows no sign change anomaly, reproducing Hall-effect behavior in clean limit type-II superconductors.

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Following the recent discovery of superconductivity at about 39 K in magnesium diboride[1] various properties of this compound have been extensively studied. Early observation of the boron isotope effect[2] clearly indicated the important role of the electron-phonon interaction in MgB_2. Subsequent measurements of specific heat,[3] ^{11}B NMR,[4] and Raman scattering[5] provided evidence for s-wave order-parameter symmetry. However, more recent studies of quasiparticle tunneling,[6,7] specific heat,[8–10] and penetration depth[11] revealed unusual features indicating a double-energy superconducting gap. Theoretical studies also give support for this scenario. In particular, the existence of two superconducting gaps in MgB_2 with a smaller one on the three-dimensional (3D) tubular network and a larger one on the 2D sheets was predicted by Liu, Mazin, and Kortus from first-principles calculations.[12]

In spite of the quite complex electronic band structure of MgB_2, results of theoretical calculations[12–15] and direct studies of the Fermi surface in angle-resolved photoemission[16] and de Haas–van Alphen[17] experiments are in good agreement. To further understand the electronic structure of MgB_2 it is crucially important to know the nature of the charge carriers in this compound. Hall-effect measurements are a powerful tool to obtain such information. Recently the Hall effect in MgB_2 has been studied using hot-pressed polycrystalline[18] and thin-film[19,20] samples. All these experiments gave a positive (holelike) sign of the Hall effect and about a one-order-of-magnitude lower value of the normal-state Hall constant, compared to low-T_c superconductors, such as Nb_3Sn and Nb_3Ge. However, the other features of the reported Hall effect of MgB_2 are rather contradictory. In particular, the T dependence of the Hall constant differed among the reported data.[18–20] Also, in the measurements below T_c Jin *et al.*[19] observed a sign change of the Hall constant before it reaches zero, while Kang *et al.* found no sign reversal in their study of the Hall effect in the mixed state.[20]

The anisotropy of the upper critical field of MgB_2 is well established now.[21–23] The availability of MgB_2 single crystals[22] opens a unique opportunity to study the anisotropy of the electrical transport properties of this compound. Here we report measurements of the in-plane $\rho_{xx} \equiv \rho_{ab}$ and out-of-plane $\rho_{zz} \equiv \rho_c$ resistivity of MgB_2 single crystals as well as the Hall effect with the magnetic field applied parallel to the c axis and along the ab planes in both the normal and superconducting states.

MgB_2 single crystals were grown as described previously.[22] Several platelike crystals of dimensions $\sim 0.5 \times 0.1 \times 0.03\ \mathrm{nm}^3$ were selected for the in-plane transport measurements, while in experiments with the current parallel to the c axis we used thicker crystals $\sim 0.2 \times 0.1 \times 0.1\ \mathrm{mm}^3$ in size. All the crystals had T_c, defined as the resistivity onset, of about 38.8 K with $\Delta T_c < 0.3$ K. Stable, low-resistance ($\sim$1–2 Ω) electrical contacts were made using gold or silver paste. For the measurements of the anisotropic resistivity, the contact configuration with two contacts on both ab planes of a crystal (sample 1) was used, as shown in the inset of Fig. 1, and ρ_{ab} and ρ_c were obtained from the Montgomery-type (MT) analysis. In our Hall-effect experiments the Hall resistivity ρ_{ij} was extracted from the antisymmetric part of the transverse voltage response under magnetic-field reversal, and the Hall constant R_{ij}^H was calcu-

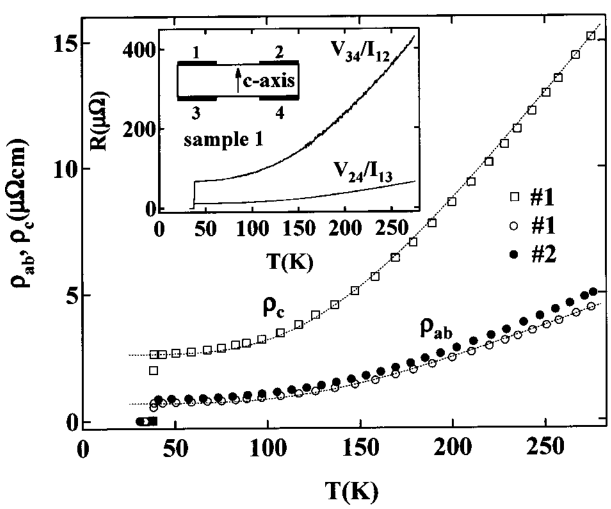

FIG. 1. Zero-field temperature dependence of the in- and out-of-plane resistivities of MgB_2 single crystals deduced from the Montgomery-type analysis for sample 1. For comparison, $\rho_{ab}(T)$ dependence obtained from the measurements with homogeneous in-plane current on sample 2 is also shown. Dotted lines represent Bloch-Grüneisen behavior as obtained from Eq. (1). Inset: Definition of contact arrangement and raw current-voltage data for sample 1.

lated as $R^H_{ij}=\rho_{ij}/H$. The in-plane Hall-effect measurements (sample 2) were performed with a homogeneous current parallel to the *ab* planes and magnetic fields directed along the *c* axis. In the Hall-effect study with *H* parallel to *ab* planes, both the out-of-plane Hall resistivity components ρ_{xz} and ρ_{zx} were obtained from the measurements with homogeneous current parallel to the *ab* planes (sample 3) and *c* axis (sample 4), respectively. The experiments were carried out in a Quantum Design physical property measurement system in magnetic fields up to 9 T with the sample mounted on a horizontal rotator. Current-voltage response was recorded using the usual low-frequency (17 Hz) ac technique with an excitation current of 0.5–1 mA within a linear regime.

The anisotropic behavior of the resistivity of the MgB_2 single crystal is illustrated in Fig. 1. The inset of Fig. 1 presents raw data obtained from the two sets of measurements with current injected along the *ab* planes (I_{12}) and parallel to the *c* axis (I_{13}). Due to the combined effect of the contact configuration, crystal geometry and resistivity anisotropy values of $R_1=V_{34}/I_{12}$ and $R_2=V_{24}/I_{13}$ are rather different, with a slightly *T*-dependent ratio $R_1/R_2\approx 6$. To extract values of the ρ_{ab} and ρ_c, we used the MT analysis.[24,25] Since the electrical terminals cover a significant portion of the sample surface, the finite contact size was taken into account. In our calculations we assumed uniform current injection within the contacts area. We also supposed that the voltage contacts did not disturb the current distribution within the sample and thus probed the averaged value of the potential at the interface between the sample and voltage terminal. Both assumptions were safely justified by the high conductivity of the crystal compared to the contact resistance.

Obtained from our analysis, results for $\rho_{ab}(T)$ and $\rho_c(T)$ are shown in the main panel of Fig. 1. Close agreement between resistivity data for samples 1 and 2 (calculated from the MT analysis and directly measured with homogeneous in-plane current distribution, respectively) gives proof of the validity of our analysis.[26] From Fig. 1 one can see the pronounced resistivity anisotropy of the MgB_2 single crystal. Just above T_c we obtain a resistivity ratio $\rho_c/\rho_{ab}=3.6\pm1.0$. The rather small and monotonic decrease of this ratio with temperature, down to $\sim$3.4 at $T=273$ K, suggests a similar temperature dependence for ρ_{ab} and ρ_c, and thus the same scattering mechanism for the in- as well as the out-of-plane charge transport. Actually, both $\rho_{ab}(T)$ and $\rho_c(T)$ for MgB_2 may be fairly well described by a Bloch-Grüneisen (BG) expression for resistivity,[19]

$$\rho=\rho_0+C^*(4\pi)^2(2T/\Theta_D)^5\int_0^{\Theta_D/2T}x^5/\sinh^2(x)dx, \quad (1)$$

where Θ_D is the Debye temperature, ρ_0 is the residual resistivity, and *C* is a proportionality constant. The dotted lines in Fig. 1 represent BG behavior as obtained from Eq. (1) with the same $\Theta_D=880$ K,[27] and different values ρ_0 of 0.69 and 2.62 $\mu\Omega$ cm, and constant *C* of 0.25 and 0.86 $\mu\Omega$ cm for ρ_{ab} and ρ_c, respectively. Thus, in agreement with theoretical calculations of the electronic structure and electron-phonon (EP) interaction in magnesium diboride[12–14] the present result demonstrates the importance of the EP scattering for both the in- and the out-of-plane resistivities.

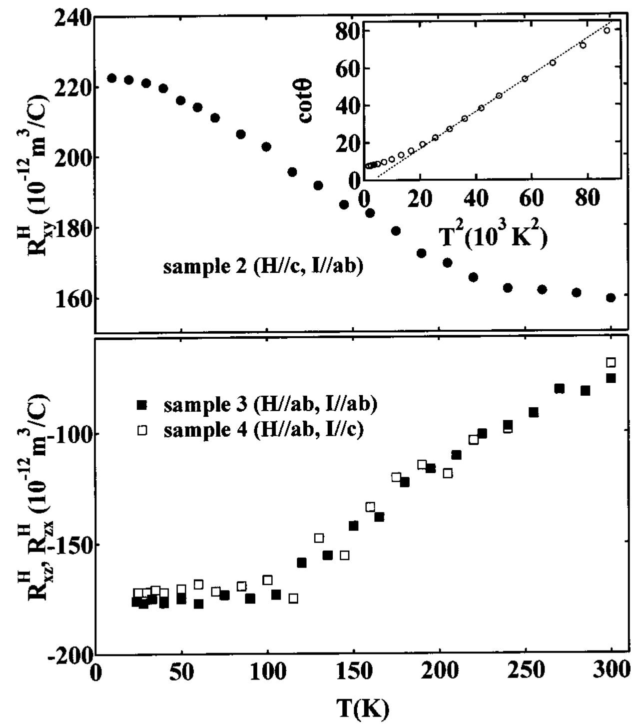

FIG. 2. The in- and the out-of-plane Hall constants, as a function of temperature in the normal state of MgB_2 single crystals (top and bottom panels, respectively). The out-of-plane Hall response was measured on two crystals with current parallel to the *ab* planes (sample 3) and I parallel to the *c* axis (sample 4). In accordance with the Onsager relation, the data for both samples demonstrate close agreement within experimental error. Inset: Temperature dependence of cot θ_H at 5 T. The line is a linear fit at intermediate temperatures of 150–220 K.

A striking anisotropy is observed in the normal-state Hall effect. Shown in Fig. 2 are the in- and the out-of-plane Hall constants vs *T*, obtained from the linear dependence of the Hall response on magnetic fields up to 9 T at various temperatures. As in the previous studies,[18–20] the in-plane Hall constant has been found to be positive, while the out-of-plane Hall response with *H* parallel to the *ab* planes shows *n*-type charge carriers. To understand this two-carrier behavior in more detail, let us first consider the Hall effect in a two parabolic band model with both electrons and holes as charge carriers. In this case the Hall constant is a sum of the contributions from each band,

$$R^H=(p\mu_p^2-n\mu_n^2)/ec(p\mu_p+n\mu_n)^2, \quad (2)$$

where *e* is the carrier charge, *c* is light velocity, *n* and *p* are the densities of electrons and holes, respectively, and μ_n and μ_p are the corresponding mobilities.[28] From Eq. (2), the positive or negative sign of the Hall constant comes from a balance of the hole and electronic terms. Thus, opposite signs of the Hall response in two magnetic-field orientations may be obtained if one suggests strongly anisotropic mobility for at least one type of carrier. The *T*-dependent behavior of both Hall constants is also expected within a two-band model, taking into account a possibility of different T dependencies of the hole and electron mobilities in Eq. (2). Actually, the situation for MgB_2 is more complicated compared to a simple two parabolic band model since the Fermi surface of this compound consists of two quasi-two-dimensional hole sheets (σ bands) and two three-dimensional light hole and electron honeycombs (π bands).[12–15] In this particular case a nearly isotropic mobility for both types of carriers from π bands as well as a strongly anisotropic mass and, thus, an anisotropic mobility for σ-band holes is expected. In fact, the results of computing the independent components of the Hall tensor for MgB_2 within a rigid-band scheme[15] show that anisotropic contribution of the hole σ states dominates in the positive in-plane Hall response, while the prevailing contribution of the electronic π band results in the n type of Hall effect with H parallel to the ab planes. Thus, our observation of two-carrier behavior is qualitatively supported by the band theory considering MgB_2 as a multiband metal. Assuming no contribution from the electrons and holes to the in- and out-of-plane transport, respectively, we can also estimate from Eq. (2) the upper limit of electron and hole densities as $n \sim 3.4\times 10^{22}$ cm^{-3} and $p \sim 2.6\times 10^{22}$ cm^{-3} at $T=40$ K. Obtained values are about one-order-of-magnitude lower than the previously reported carrier density for bulk and thin-film MgB_2 samples.[18–20] This difference does not look surprising, since the apparent Hall coefficient derived from the measurements on polycrystalline samples with randomly oriented grains could represent a sum of the in- and out-of-plane Hall responses of opposite polarities, thus, resulting in overestimated carrier density.

We would also like to point out that the different signs of the in- and out-of-plane Hall constants in MgB_2 resemble the Hall effect in $YBa_2Cu_3O_{7-\delta}$ with p- and n-type Hall responses obtained in studies with H parallel to the c axis and ab planes, respectively.[29,30] However, this similarity does not extend to the T dependence of the Hall effect in MgB_2 and the high-T_c superconductors (HTS). In particular, studies of the Hall effect in various HTS revealed an anomalously strong T dependence of the in-plane Hall constant, which just above T_c can be turned into a simple T^2 dependence of the cotangent of the Hall angle, cot $\theta_H=\rho_{xx}/\rho_{xy}$ (for a review, see Ref. 31). According to Anderson,[32] this unusual behavior of the Hall effect in HTS was interpreted as a result of the existence of two distinct relaxation time scales. On the contrary, for MgB_2, cot $\theta_H(T)$ does not show a T^2 dependence in a broad temperature range as obtained from our resistivity and Hall-effect measurements (see inset in the upper panel of Fig. 2).[33] Furthermore, the T dependence of the Hall constant in MgB_2 and HTS seems to be of completely different origins. As mentioned above, in a multiband metal, such as MgB_2, the T dependence of the Hall constant may come from the different T dependencies of the hole and electron mobilities. Such a possibility was recently suggested in a model of electric transport in MgB_2 based on the assumption of a large difference in the scattering rate of the σ and π bands and extremely small $\sigma\pi$ scattering.[34]

Finally, we present results of the Hall-effect measurements in the mixed state of a MgB_2 single crystal. Shown in Fig. 3 are T dependencies of the in- and out-of-plane longitudinal and Hall resistivities. As reported previously[23] ρ_{xx} exhibits a remarkable broadening of the superconducting transition in a magnetic field. Measured simultaneously, ρ_{xy} was found to be positive in the entire transition region, and with decreasing temperature monotonically decreased to zero. Data for the out-of-plane Hall effect display a very similar behavior, except for the negative sign of the out-of-plane Hall constant, a smaller transition width, and a higher transition temperature in a magnetic field of the same magnitude. In striking contrast to the Hall voltage sign reversal previously reported for MgB_2 films[19] our results for both the in- and out-of-plane Hall effects do not show sign change. However, as we already mentioned, the anomalous Hall-effect behavior in polycrystalline MgB_2 samples may have an extrinsic origin reflecting a possible mixture of the in- and out-of-plane Hall responses of opposite polarities.

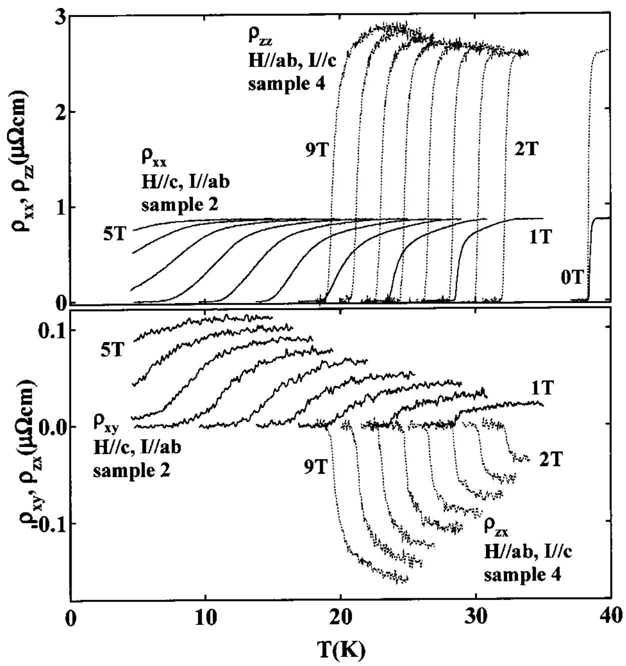

FIG. 3. Upper panel: The mixed-state temperature dependence of ρ_{xx} and ρ_{zz} at various magnetic fields of (from right to left) 0, 1, 1.5, 2, 2.5, 3, 3.5, 4, 4.5, and 5 T parallel to the c axis and of (from right to left) 0, 2, 3, 4, 5, 6, 7, 8, and 9 T parallel to the ab planes, respectively. Lower panel: The in- and out-of-plane Hall resistivities at the same fields.

In conventional superconductors the Hall-effect sign change anomaly near T_c was reported for moderately clean superconductors with a ratio $l/\xi_0=0.5\div 5$, where l is the electron mean free path, and ξ_0 is the coherence length, while a sign reversal does not occur in either the clean ($l \gg \xi_0$) or dirty ($l \ll \xi_0$) limits (see Ref. 35, and references therein). For MgB_2, the in- and out-of-plane coherence lengths were found to be $\sim$68 and $\sim$23 Å, respectively.[23] Using data for anisotropic resistivity and carrier density obtained from our normal-state measurements, and the Fermi velocity of 4.9×10^7 cm/s parallel to the ab planes and of 4.76×10^7 cm/s along the c axis,[13] we estimate the corresponding l to be $\sim$700 and $\sim$180 Å just above T_c, and, thus, $l/\xi_0 \sim 10$ for both directions. From this analysis we can conclude that the absence of the Hall-effect sign change in MgB_2 is in good agreement with the empirical correlation between microscopic material parameters and the mixed-state Hall-effect behavior reported for type-II superconductors.[35]

In summary, the in- and out-of-plane electrical transport properties of MgB_2 single crystals have been studied. We found substantial resistivity anisotropy with a resistivity ratio $\rho_c/\rho_{ab}\approx 3.5$. Both ρ_{ab} and ρ_c display similar T dependencies described by a BG expression as a first approximation, thus indicating a predominant contribution of the EP interaction to the in- as well as out-of-plane charge transport in MgB_2. Measurements of the normal-state Hall effect with H parallel to the ab planes and the c axis revealed the presence of both types of charge carriers. In agreement with the theoretical prediction this result clearly demonstrates the multiband electronic structure of MgB_2. In the mixed state the in- as well as out-of-plane Hall constants display no sign change anomaly reproducing the Hall-effect behavior in clean limit type-II superconductors.

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