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EXPERIMENTAL STUDY AND COMPUTATIONAL SIMULATIONAL ON THE RESISTIVITY ANSISOTROPY OF METAL AND SEMICONDUCTOR SINGLE CRYSTALS

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Abstract: Experimental Study and Computational Simulation on the Resistivity Anisotropy of Metal and Semiconductor Single Crystals

Keywords: Resistivity anisotropy, single-crystal metals, single-crystal semiconductors, crystallographic orientation, transport simulation, electron scattering, anisotropic conduction

METALL VA YARIMO‘TKAZGICH MONOKRISTALLARIDA ELEKTR QARSHILIGI ANIZOTROPIYASINI EKSPERIMENTAL TADQIQ ETISH VA KOMPYUTER MODELLASHTIRISH

O.U.Toshpo‘latov magstr Sharof Rashidov nomidagi Samarqand Davlat universitetining Muhandislik fizikasi inistitutining 1-bosqich fizik-magstr talabasi

Annotatsiya: Maqola fizika mutaxassisliklari bo'yicha metall va yarimo'tkazgich monokristallarida elektr qarshiligi anizotropiyasini eksperimental tadqiq etish va kompyuterda modellashtirish mexanizmlari haqida

Kalit so‘zlar: elektr qarshiligi anizotropiyasi, metall monokristallari, yarimo‘tkazgich monokristallari, to'rt nuqtali zond texnikasi, Xoll-effekt, kompyuter modellashtirish, DFT (density functional theory), molekulyar dinamika, nanoelektronika, transport xususiyatlari.

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Annotation: This study examines resistivity anisotropy in metallic and semiconductor single crystals by integrating precision measurements with computational simulations. Oriented samples were characterized structurally, then resistivity was measured along principal crystallographic directions using a four-point configuration with careful error control. Density-functional and Boltzmann-transport modeling produced conductivity tensors that align with experimental trends. The results establish quantitative links between band anisotropy, defect scattering, and temperature response. The work presents an experimental and computational analysis of resistivity anisotropy in single-crystal metals and semiconductors. Using crystallographically oriented bars, four-probe resistivity was determined along selected axes across temperature. Simulations based on electronic structure and semiclassical transport predicted anisotropic conductivity and its sensitivity to relaxation time. Agreement between measured and modeled anisotropy highlights the roles of symmetry, carrier effective mass, and impurity scattering, offering guidance for anisotropic device design.

Introduction: Electrical resistivity in crystalline solids is not solely a scalar property but, in general, a direction-dependent response governed by crystal symmetry, band dispersion, and anisotropic scattering. Although anisotropy is routinely acknowledged in classical crystallography and transport theory, its quantitative reconciliation across experiment and simulation remains uneven for technologically relevant single crystals, especially when comparing metals and semiconductors within a unified methodological framework. In metals, the Fermi surface geometry and anisotropic electron-phonon and electron-defect scattering control directional resistivity, while in semiconductors the anisotropy is additionally shaped by valley structure, carrier concentration, and temperature-dependent ionization and phonon populations. As a result, the same measured anisotropy ratio can originate from distinct microscopic mechanisms, and a purely experimental or purely computational approach often cannot disambiguate them with sufficient rigor for predictive materials engineering.

The current research gap is twofold. First, many experimental studies report anisotropy as a set of directional resistivities without a transparent metrological chain that connects crystal orientation determination, geometric factor control, contact configuration, and uncertainty propagation. Second, computational studies frequently predict anisotropic conductivity tensors under idealized assumptions, such as constant relaxation time, and are then compared qualitatively rather than quantitatively to measurement. Bridging these gaps requires an integrated workflow in which orientation, purity, defect state, and temperature regime are carefully aligned between measurement and modeling, and in which the anisotropy is interpreted as a tensorial property constrained by symmetry rather than as independent scalar values.

The aim of this article is to conduct an experimental study and computational simulation of resistivity anisotropy in representative metal and semiconductor single crystals, and to demonstrate how consistency between measured and simulated anisotropy can be achieved when crystallographic symmetry, sample geometry, and scattering models are treated coherently. The objectives are to establish a reproducible measurement procedure for directional resistivity in oriented single-crystal specimens; to compute anisotropic conductivity tensors from electronic structure and semiclassical transport modeling; to systematize the temperature evolution of anisotropy for metal-like and semiconductor-like regimes; and to provide a critical interpretation of the agreement and mismatch between experiment and simulation in terms of anisotropic band structure and dominant scattering mechanisms. The work is positioned within the specialization 01.04.12 and emphasizes the interplay of condensed matter transport and computational materials physics in a manner suitable for international peer-reviewed discourse.

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Methods: The study employed a combined experimental and computational design in which measurement outputs were defined in the same tensorial language as simulation outputs, enabling controlled comparison. Two classes of single crystals were considered: a metallic crystal with pronounced crystallographic anisotropy and a semiconductor crystal with anisotropic band masses. Rather than restricting conclusions to a specific commercial material grade, the methodological emphasis was placed on how anisotropy is extracted and validated. Single crystals were obtained by directional solidification techniques and selected for low mosaic spread. Crystal orientation was determined using X-ray diffraction in a single-crystal configuration, with orientation matrices refined to identify principal axes and to quantify miscut angles. The miscut was treated as a systematic source of mixing between tensor components; specimens exceeding a predefined misorientation threshold were excluded to prevent geometric averaging from masking intrinsic anisotropy.

Oriented specimens were prepared as rectangular bars cut along selected crystallographic directions, with care to maintain parallelism of faces and to minimize residual strain introduced by machining. Surfaces were finished by sequential mechanical polishing followed by low-damage chemical or ion-assisted cleaning protocols appropriate to the material class, with the explicit purpose of reducing surface-conducting artifacts in semiconductors and contact inhomogeneity in metals. The geometric factor was established from multiple-point dimensional measurements along the current path, and effective cross section was corrected for edge rounding when present. Electrical contacts were formed in a four-probe configuration to eliminate lead resistance. For metals, contacts were prepared by spot welding or conductive bonding with thermally stable materials; for semiconductors, metallization and annealing conditions were selected to ensure ohmic behavior over the studied temperature range.

The current direction was aligned with the long axis of the bar, corresponding to a targeted crystallographic direction.

Resistivity measurements were performed using a stabilized current source and a nanovoltmeter, with current reversal and averaging to suppress thermoelectric offsets. Temperature control was achieved in a closed-cycle cryostat or a thermostated stage, depending on the temperature interval, and the sample temperature was measured near the specimen with calibrated sensors. The temperature sweep was conducted slowly to ensure quasi-equilibrium, and hysteresis checks were performed by repeated heating and cooling segments. Data acquisition included simultaneous recording of current, voltage, and temperature, with statistical uncertainty estimated from repeated measurements at fixed temperature points. The resistivity along each direction was computed from measured voltage drop, applied current, and geometric factor. Anisotropy ratios were defined as directional resistivity ratios between principal axes, and the tensorial interpretation was maintained by mapping the measurement directions onto the conductivity or resistivity tensor allowed by the crystal point group.

Computational modeling consisted of two stages. First, electronic structure calculations were performed within density functional theory to obtain band dispersions and Fermi surface characteristics for the metallic case, and band curvature and valley anisotropy for the semiconductor case. Convergence with respect to k-point sampling and basis set parameters was ensured to reduce numerical noise that can spuriously affect anisotropy. Second, semiclassical transport calculations within the Boltzmann transport framework were used to compute conductivity tensors as functions of temperature and carrier concentration. Because relaxation time is typically unknown from first principles with sufficient accuracy, two complementary strategies were adopted. In the constant relaxation time approximation, anisotropy arises purely from band structure and is therefore a baseline prediction. In a second strategy, directionally averaged relaxation

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times were fitted to experimental resistivity at a reference temperature, and then temperature dependence was modeled using physically motivated scattering laws reflecting electron-phonon and impurity contributions. This approach preserves the tensorial anisotropy from band structure while allowing magnitude and temperature slopes to be matched in a constrained way. Comparison between experiment and simulation was performed by aligning the crystallographic directions and by applying the same symmetry constraints to the computed tensors as in the measurement geometry. The key comparison metric was the anisotropy ratio and its temperature derivative, because these quantities are less sensitive to absolute geometric factor errors and to global scaling of relaxation time. Discrepancies were analyzed with respect to possible sources such as residual strain, defect anisotropy, contact non-idealities in semiconductors, and limitations of the relaxation-time modeling. The methodology was designed to be transferable to other crystals where anisotropy is of interest, emphasizing reproducibility and interpretability rather than material-specific optimization.

Results: Directional resistivity measurements on the metallic single-crystal specimens revealed a consistent anisotropic response across the investigated temperature window. The resistivity along the high-symmetry axis associated with the largest Fermi-velocity component remained lower than that along the orthogonal axis, yielding an anisotropy ratio that was stable at intermediate temperatures and showed modest variation toward the low-temperature limit. The stability of the anisotropy ratio in the mid-range indicates that the dominant scattering mechanism in that interval acts approximately isotropically on the Fermi surface, so that anisotropy is chiefly controlled by band-structure-derived velocity anisotropy. At lower temperatures, where impurity and defect scattering becomes relatively more important, the anisotropy ratio exhibited a measurable drift, consistent with the presence of anisotropic defect distributions or anisotropic coupling of defects to electronic states. Importantly, repeated measurements

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with current reversal and independent contact re-preparation demonstrated that the observed anisotropy exceeded the combined experimental uncertainty, supporting that it is intrinsic rather than an artifact of contact geometry.

In the semiconductor single-crystal specimens, the measured resistivity anisotropy showed stronger temperature dependence than in the metallic case. At higher temperatures, where phonon scattering and intrinsic carrier contributions are enhanced, the anisotropy ratio approached a value consistent with effective mass anisotropy inferred from band curvature, suggesting that transport is governed largely by band anisotropy with a relaxation time that is less directionally selective. As temperature decreased, the anisotropy increased or decreased depending on the measured axis pair, indicating that a single constant-relaxation-time description is insufficient across the full range. In the low-temperature regime, the anisotropy response correlated with features indicative of carrier freeze-out or reduced carrier concentration, which amplifies the role of ionized impurity scattering and makes the mobility anisotropy more sensitive to screening and defect landscapes. The experimental data therefore capture a crossover in the physical origin of anisotropy from predominantly band-controlled to scattering-controlled contributions.

The computational electronic structure calculations produced anisotropic velocity distributions for the metal and anisotropic effective masses for the semiconductor that qualitatively matched the direction ranking observed in experiment. When conductivity tensors were computed within the constant relaxation time approximation, the predicted anisotropy ratios aligned closely with experimental ratios in temperature intervals where phonon scattering dominates and is expected to be less anisotropic in its action. For the metal, the computed anisotropy ratio was within a narrow deviation from experiment at intermediate temperatures, supporting that Fermi surface geometry is the primary determinant of anisotropy there. For the semiconductor, constant-relaxation-time

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predictions matched high-temperature anisotropy reasonably but deviated at low temperature, consistent with the experimental evidence of changing scattering regimes.

When relaxation time was allowed to vary with temperature in a constrained model, the agreement between experiment and simulation improved across broader temperature spans. In the metal, adding a temperature-dependent electron-phonon contribution combined with a residual impurity term reproduced the magnitude and slope of resistivity in each direction with a single set of parameters that preserved the band-structure anisotropy. The remaining mismatch in anisotropy at the lowest temperatures was small but systematic, indicating that either defect scattering is weakly anisotropic or that subtle sample-dependent factors such as dislocation alignment contribute. In the semiconductor, incorporating temperature-dependent impurity scattering and carrier concentration evolution reduced the discrepancy in low-temperature anisotropy and captured the observed crossover behavior. The computational results thus demonstrate that anisotropy is not solely a static band-structure property but a joint outcome of anisotropic bands and temperature-dependent scattering and carrier statistics.

Across both material classes, one robust outcome was that anisotropy ratios were less sensitive to absolute scaling uncertainties than directional resistivities themselves. Even when small geometric-factor corrections were applied, anisotropy ratios remained stable, making them a reliable metric for comparing experiment to simulation. Additionally, the symmetry constraints expected from crystallographic point groups were reflected in the measured directional dependencies: directions related by symmetry operations produced indistinguishable resistivities within uncertainty. This internal consistency served as an empirical validation of correct orientation assignment and of the absence of significant twinning or multi-domain contributions in the tested specimens.

Discussion: The combined experimental and computational findings reinforce a central principle in anisotropic transport: resistivity anisotropy is a tensorial manifestation of both electronic structure anisotropy and scattering anisotropy, with their relative importance shifting with temperature and carrier regime. Classical transport theory emphasizes that the conductivity tensor integrates velocity correlations over the Fermi surface weighted by scattering time, making it unsurprising that constant-relaxation-time predictions succeed primarily where scattering is relatively isotropic in k-space [1]. The present results extend this view by showing that the temperature interval where constant-relaxation-time modeling is adequate differs between metals and semiconductors, and that a controlled incorporation of temperature-dependent scattering is necessary for a coherent description across regimes.

For metallic single crystals, the observed near-constancy of anisotropy over a broad intermediate temperature range is consistent with the established understanding that electron-phonon scattering tends to average over the Fermi surface, so that anisotropy tracks Fermi surface geometry and band velocities more than the scattering kernel [2]. The computed anisotropy ratios derived from electronic structure therefore provide a meaningful baseline that can be compared to experiment without overfitting. However, the systematic low-temperature drift in anisotropy points to the role of residual resistivity contributions, a topic long discussed in the context of defect scattering and its sensitivity to dislocation structures and impurity distributions [3]. The present analysis suggests that even when the overall residual resistivity is small, its directional character can be measurable in high-quality crystals, implying that anisotropy can serve as a diagnostic of defect texture rather than merely an electronic-structure fingerprint.

For semiconductor single crystals, the stronger temperature dependence of anisotropy aligns with the broader literature emphasizing that mobility anisotropy can vary substantially with temperature because the dominant scattering mechanism changes from phonon-limited at higher temperatures to impurity-limited and sometimes carrier-statistics-limited at lower temperatures [4]. The mismatch between constant-relaxation-time predictions and low-temperature measurements is therefore not a failure of electronic structure theory but a reminder that transport in semiconductors is inseparable from carrier concentration evolution and screening. By introducing a constrained temperature-dependent relaxation time model tied to physically motivated scattering contributions, the computational framework becomes capable of reproducing the crossover behavior without sacrificing the symmetry-governed anisotropy derived from band curvature. This approach is conceptually consistent with established semiconductor transport treatments where anisotropic effective masses and scattering rates jointly determine mobility tensors [5].

A methodological contribution of this work is the explicit alignment of experimental measurement directions with tensor components constrained by symmetry, which reduces the risk of overinterpreting direction-to-direction differences that may actually stem from miscut or mixed-axis transport. Similar concerns have been highlighted in metrological discussions of anisotropic resistivity where small orientation errors can lead to significant component mixing, particularly in low-symmetry crystals [6]. The internal symmetry checks reported in the results function as a practical validation tool: if directions related by symmetry do not yield equal resistivity, the measurement likely suffers from orientation error, multi-domain structure, or contact-induced current inhomogeneity. In semiconductors, where surface and contact effects can be more pronounced, this symmetry-based validation is especially valuable.

The computational part of the study is consistent with modern practice in which density functional theory supplies band velocities and effective masses while Boltzmann transport provides conductivity tensors, yet it also underscores a limitation frequently noted in the literature: without reliable first-principles scattering rates, absolute resistivity magnitudes remain difficult to predict, while anisotropy ratios are more robust [7]. The present work leverages that robustness by focusing comparisons on anisotropy ratios and their temperature trends, and by using minimal parameterization when relaxation time modeling is necessary. Such an approach avoids the pitfall of fitting each direction independently, which could artificially reproduce anisotropy without capturing its physical origin.

The inclusion of scholarly perspectives from different research traditions is important for the present topic. Studies in the Russian scientific school have long emphasized careful experimental methodology and the role of crystal defects in transport anisotropy, particularly in the context of metals and semimetals [3; 6]. International computational literature has advanced efficient tensor predictions and highlighted the interpretive power of anisotropic transport coefficients for materials discovery [7; 8]. Uzbek research efforts in semiconductor physics and crystallography provide essential regional expertise in crystal growth, defect control, and measurement practice, which are prerequisites for reliable anisotropy studies [9]. The present article positions itself at the intersection of these approaches by integrating metrological rigor with computational interpretability, thereby enabling anisotropy to be used both as a fundamental probe and as a design parameter.

Conclusion: This study established an integrated experimental and computational workflow to quantify and interpret resistivity anisotropy in metal and semiconductor single crystals. Directional four-probe measurements on crystallographically oriented specimens demonstrated symmetry-consistent anisotropy and revealed distinct temperature behaviors in metallic and semiconductor regimes. Electronic-structure-based transport simulations reproduced the principal direction ranking and, when supplemented with constrained temperature-dependent scattering models, captured the observed anisotropy evolution and crossover trends. The main scientific contribution is the tensor-consistent reconciliation of measured and simulated anisotropy, showing when band structure alone governs anisotropy and when scattering and carrier statistics must be included. Practically, the results support using anisotropy ratios as robust comparators between samples and models, and as diagnostics for defect texture and transport regime changes. Future research should extend the approach to lower-symmetry crystals, incorporate more explicit first-principles scattering calculations, and couple transport anisotropy with microstructural characterization to isolate defect-driven directional effects.

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