Resistivity scaling in CuTi determined from transport measurements and first-principles simulations

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The resistivity size effect in the ordered intermetallic CuTi compound is quantified using in situ and ex situ thin film resistivity ρ measurements at 295 and 77 K, and density functional theory Fermi surface and electron-phonon scattering calculations. Epitaxial CuTi(001) layers with thickness d = 5.8-149 nm are deposited on MgO(001) at 350 °C and exhibit ρ vs d data that are well described by the classical Fuchs and Sondheimer model, indicating a room-temperature effective electron mean free path λ = 12.5 ± 0.6 nm, a bulk resistivity ρ₀ = 19.5 ± 0.3 μΩ cm, and a temperature-independent product ρ₀λ = 24.7 × 10⁻¹⁶ Ω m². First-principles calculations indicate a strongly anisotropic Fermi surface with electron velocities ranging from 0.7 × 10⁵ to 6.6 × 10⁵ m/s, electron-phonon scattering lengths of 0.8-8.5 nm (with an average of 4.6 nm), and a resulting ρ₀ = 20.6 ± 0.2 μΩ cm in the (001) plane, in excellent agreement (7% deviation) with the measurements. However, the measured ρ₀λ is almost 2.4 times larger than predicted, indicating a break-down of the classical transport models. Air exposure causes a 6-30 % resistivity increase, suggesting a transition from partially specular (p = 0.5) to completely diffuse surface scattering due to surface oxidation as detected by x-ray photoelectron spectroscopy. Polycrystalline CuTi layers deposited on SiO₂/Si substrates exhibit a 001 texture, a grain width that increases with d, and a 74-163 % larger resistivity than the epitaxial layers due to electron scattering at grain boundaries. The overall results suggest that CuTi is a promising candidate for highly scaled interconnects in integrated circuits only if it facilitates liner-free metallization.

I. INTRODUCTION

Copper has been the primary interconnect metal in integrated circuits for the last two decades since it replaced aluminum owing to its higher conductivity and resistance against electromigration. However, the continued downscaling of feature sizes and the proportional decrease in the interconnect line widths¹⁻⁴ below the electron-phonon scattering mean free path causes a steep increase in the resistivity due to increased electron scattering at surfaces and grain boundaries.⁵,⁶ This represents a major challenge for the further downscaling because the increased resistivity and decreased cross-sectional area of interconnect lines causes a resistance-capacitance (RC) delay which limits device speed. The RC delay is exacerbated by the need for liner and barrier
layers which suppress Cu diffusion into the surrounding dielectric but occupy an increasing portion of the trench volume and cause a corresponding resistance increase. Therefore, there is an urgent need for a new interconnect conductor material that exhibits a low resistivity scaling and requires no or much thinner barrier layers.

The search for Cu replacement metals has focused on materials which have a low product of the bulk resistivity \( \rho \) times the electron mean free path \( \lambda \). This \( \rho \lambda \) product is a metric to quantify the resistivity scaling because it acts as a pre-factor in both the Fuchs and Sondheimer (FS) model\(^9\)\(^{10}\) for surface scattering and the Mayadas and Shatzkes (MS) model\(^11\) for grain boundary scattering. Correspondingly, metals with a low \( \rho \lambda \) are expected to be most conductive in the limit of narrow wires and/or small grain size. Elemental metals have been explored extensively using both computational\(^12\)-\(^14\) and experimental methods yielding measured \( \rho \lambda \) values (in units of \( 10^{-16} \ \Omega \text{m}^2 \)) of 5.1 for Ru,\(^15\) 10.8/18.9 for W,\(^16\) 12.2 for Co,\(^17\) 4.5 for Rh,\(^18\) 6.3 for Ag,\(^19\) 18.3 for Ni,\(^20\) 33 for Nb,\(^21\) and 3.8 for Ir,\(^22\) suggesting that some metals have the potential to outperform Cu, which has a measured \( \rho \lambda = 6.6 \times 10^{-16} \ \Omega \text{m}^2 \). More recently, the materials search has been expanded to conductive compounds including layered MAX-phases materials\(^23\),\(^24\) where anisotropic conduction may facilitate transport along narrow lines\(^7\),\(^25\) and intermetallic compounds including aluminides\(^26\) such as NiAl\(^27\),\(^28\) and CuAl\(^29\),\(^30\) or also CuMg\(^31\) where high cohesive energies suggest good electromigration performance and good stability against diffusion into the dielectric, promising metallization without liner and/or barrier layers\(^32\),\(^33\) with an associated substantial conductance benefit. CuTi is another alternative compound conductor for narrow interconnect lines with a predicted cohesive energy of 4.33 eV/atom,\(^34\) a melting point of 898 °C,\(^35\) but without a known resistivity and resistivity size effect.

In this paper, we measure the CuTi resistivity and its size effect. For this purpose, resistivity vs thickness data from epitaxial CuTi(001) layers is analyzed with the FS model to determine the bulk resistivity and effective electron mean free path. Polycrystalline layers are used to quantify the resistance contribution from grain boundary scattering. The resistance difference from in situ measurements and air exposed samples provides insight into the decrease in surface scattering specularity upon surface oxidation. The overall results indicate that the bulk resistivity of CuTi is an order of magnitude larger than for copper and the effective electron mean free path is three times smaller than for copper. Our first-principles calculations indicate a smaller resistivity scaling than observed experimentally, with a predicted ballistic conductance of \( 1.05 \times 10^{-15} \ \Omega^{-1}\text{m}^2 \), a \( \rho \lambda = 9.56 \times 10^{-16} \ \Omega \text{m}^2 \) and a room-temperature electron mean free path of 4.6 nm (~ 6.7 times smaller than that of Cu). Nevertheless, both experiments and simulations show that CuTi exhibits no intrinsic conductance advantage over Cu and may become promising for narrow interconnect lines only if its higher stability facilitates liner-free interconnects.

II. METHODS

CuTi thin films were deposited in a three-chamber ultrahigh vacuum DC magnetron sputtering system with a base pressure < 10^{-9} Torr.\(^36\)-\(^38\) The substrates were
polished MgO(001) or p-type Si wafers with a 100-nm-thick thermally grown SiO$_2$ layer. They were ultrasonically cleaned in trichloroethylene, acetone, iso-propyl alcohol, and de-ionized water for 15 min each. MgO(001) wafers were degassed in vacuum in the deposition system at 1000 °C for one hour. The temperature was adjusted to 350 °C for deposition in 3 mTorr 99.999% pure Ar, using constant powers of 60 and 50 W applied to 51-mm-diameter Cu (99.999%) and Ti (99.995%) targets which were sputter cleaned for 10 minutes prior to deposition. The targets were facing a continuously rotating substrate at 9 cm with a 45° tilt, yielding a deposition rate of 9.6 nm/min. The deposition time was adjusted to obtain various CuTi film thicknesses $d = 5.8 - 149$ nm on both MgO(001) and SiO$_2$/Si. After deposition, the samples were allowed to cool in vacuum to room temperature for approximately 12 h, followed by transfer in vacuum to the analysis chamber for electrical transport measurements with an *in situ* linear four-point probe with a 1.0 mm inter-probe spacing operated with 1-100 mA. Subsequently, the samples were transferred to a load-lock that was vented with dry N$_2$, removed from the deposition system and submerged into liquid nitrogen within 2 s to minimize oxygen exposure prior to cryogenic transport measurements which were performed with a similar four-point probe with both sample and measurement tips immersed in liquid N$_2$. The samples were subsequently warmed to room temperature by continuously blowing dry N$_2$ gas to the top surface to minimize water condensation, followed by *ex situ* resistivity measurements at room temperature. The resistivity was determined from the measured resistance using correction factors for sample geometry$^{39}$ and layer thickness measured by X-ray reflectivity (XRR).

X-ray diffraction (XRD) and XRR characterization was conducted using a Panalytical X’pert PRO MPD system with a Cu Kα source. Symmetric $\theta$-2$\theta$ scans and $\omega$ rocking curves were obtained using a parabolic mirror which yields a source divergence $<$0.055°. XRD $\phi$-scans were acquired with fixed $2\theta$ values and $\chi$ tilts to detect asymmetric reflections from the substrate and CuTi(001) layer, using a point focus optics combined with a polycapillary X-ray lens that provides a quasi-parallel Cu Kα beam with a divergence $<$0.3°. Asymmetric reciprocal space maps around the CuTi 204 reflection were obtained using an X-ray hybrid mirror Ge(220) two-bounce monochromator which yields a Cu K$_{\text{α1}}$ beam ($\lambda = 1.5406$ Å) with a 0.0068° divergence and taking advantage of parallel acquisition with all 256 channels of a PW3018/00 PIXcel solid-state line detector in scanning mode. XRR patterns were obtained using parallel x-rays from the parabolic mirror and were analyzed using the Panalytical X’Pert Reflectivity software based on the recursive theory of Parratt.$^{40}$ The XRR oscillations for layers with $d > 100$ nm could not be resolved. Thus, the thickness of these samples was determined from the deposition rate, as measured from thinner samples. Atomic force microscopy (AFM) was done using a Digital Instruments Multimode III-a tool with a silicon cantilever with a 4 μm tip radius and a resonance frequency of 320 kHz. $5 \times 5$ μm$^2$ images with a $512 \times 512$ pixel resolution were acquired in tapping mode.

XPS analyses were performed in a PHI 5000 Versaprobe system using Al Kα radiation (1486.6 eV) and a hemispherical analyzer with an eight-channel detector. The
sample surfaces were sputter etched using a 3 keV 2 mA Ar⁺ beam incident at 45° relative to the surface normal over a 1 mm² area, yielding a 9.2 nm/min sputter rate. Ion beam sputtering was done in 15 s steps, corresponding to etching 2.3 nm per step, followed by acquisition of high-resolution spectra of Ti 2p, Cu 2p, Mg 1s and O 1s peaks using a pass energy of 50 eV and a step size of 0.2 eV. A 1.2 eV electron flood gun in conjunction with a low-energy (7 eV) ion neutralizer were used to compensate for possible charge buildup due to photoemission. The composition was determined from the relative area under the curve for each peak after Shirley background subtraction and using the sensitivity factors within the PHI MultiPak software package. Rutherford Backscattering Spectrometry (RBS) was conducted with a Dynamitron ion accelerator using a 2 MeV alpha-particle beam. The 2-MeV He⁺ ions were collimated to 2 × 2 mm² by a series of apertures. Backscattered particles were collected in a high-vacuum (~ 10⁻⁷ torr) chamber with a Si surface barrier detector positioned at a scattering angle of 166°. The beam current of ~ 5 nA was measured by a beam chopper. Energy calibration was done with a gold thin film standard and the spectra were analyzed with the SIMNRA simulation software.

First-principles calculations were performed using density functional theory (DFT) as implemented in the open-source planewave DFT package JDFTx. The electronic structure was calculated using the non-relativistic Garrity-Bennett-Rabe-Vanderbilt (GBRV) pseudopotentials and the revised Perdue-Burke-Ernzerhof (PBEsol) generalized gradient approximation (GGA) exchange-correlation functional. The self-consistent calculations used an electronic planewave cutoff of 1224.5 eV, a charge density cut-off of 12245 eV, an \(8 \times 8 \times 8\) \(k\)-point sampling, a \(2 \times 2 \times 2\) \(q\)-point sampling, and a Fermi smearing of 0.272 Hartrees. The initial structure of CuTi as obtained from the Materials Project database is relaxed using the limited-memory Broyden-Fletcher-Goldfarb-Shanno (L-BFGS) optimization algorithm which yields a tetragonal cell with lattice parameters: \(a = b = 3.09\) Å and \(c = 5.83\) Å. Next, the calculated electronic states, phonon modes and electron-phonon matrix elements are transformed from the planewave basis set to the maximally localized Wannier functions basis set. This enables Wannier interpolation to obtain a dense sampling of \(k\)- and \(q\)-meshes for the calculation of the Fermi surface, \(\rho_\omega\) tensor and bulk resistivity \(\rho_0\). The Fermi surface and the \(\rho_\omega\) tensor are computed using a sampling of \(256 \times 256 \times 256\) and \(4096 \times 4096 \times 4096\) \(k\)-points, respectively, with a Fermi smearing of 0.0027 eV. Please refer to our previous reports for more details on the \(\rho_\omega\) calculations and the methodology used for electron-phonon scattering and bulk resistivity calculations.

III. RESULTS

Figure 1 shows representative XRD results from a 33.3-nm-thick epitaxial CuTi(001)/MgO(001) layer (red) and from a 44.3-nm-thick polycrystalline CuTi/SiO₂/Si(001) layer (blue). The \(\theta-2\theta\) pattern (red) in Fig. 1(a) shows a sharp peak at 42.93° ascribed to the MgO 002 substrate reflection and layer peaks at 14.92° and 62.46° attributed to the CuTi 001 and the CuTi 004 reflections, respectively. No other peaks can be detected over the entire measured 2\(\theta\) = 10-80° range, indicating an ordered
CuTi compound with no detectable misoriented grains or secondary phases, despite the narrow composition range for the CuTi phase in the Cu-Ti phase diagram. We note that no peaks for the CuTi 002 and 003 reflections can be detected, consistent with the 30 and 110 times weaker expected intensity, respectively. The CuTi 001 peak position corresponds to an out-of-plane lattice constant \( c = 5.937 \) Å while the CuTi 004 reflection yields \( c = 5.947 \) Å. Both values are slightly larger than the reported \( c = 5.919 \) Å, suggesting a small or negligible (< 0.5%) strain as discussed below. The CuTi 001 peak width in \( 2\theta \) indicates a vertical x-ray coherence length of 39 nm. This is close to the layer thickness of 33.3 nm and indicates a negligible peak broadening associated with crystalline defects. We note that plotting the pattern with a larger \( 2\theta \)-resolution reveals that the MgO 002 substrate peak is a double-peak feature (at 42.93° and 43.05°) caused by Cu Kα1 and Kα2 x-rays while the doublet cannot be resolved for the layer peaks. The blue curve in Fig. 1(a) is from a polycrystalline CuTi layer deposited on amorphous SiO2/Si(001) using the same deposition conditions used for epitaxial layer growth. It exhibits a Si 004 substrate doublet peak at 69.13/69.33° and CuTi 001 and 004 reflections at \( 2\theta = 14.91° \) and 62.54°. No other peaks can be detected, indicating a strong CuTi 001 preferred orientation along the growth direction. The CuTi 001 and 004 peak positions match those from the epitaxial layers within an experimental accuracy of 0.6 %, suggesting negligible compositional or strain variations. The peak intensities are 26 and 35 times weaker than for the epitaxial CuTi(001), indicating a reduced crystalline alignment or a higher density of crystalline defects for the polycrystalline layer deposited on SiO2/Si(001).

Fig. 1(b) shows an \( \omega \)-rocking curve of the CuTi 001 reflection from the 33.3-nm-thick epitaxial CuTi(001) layer. It exhibits a full-width at half-maximum (FWHM) of 1.3°, confirming the strong crystalline alignment of the CuTi[001] axis perpendicular to the MgO(001) surface. The corresponding in-plane x-ray coherence length is 26 nm. This value which indicates the degree of mosaicity is similar to what has been reported for other epitaxial metal films deposited onto MgO(001) including W(001) with 33 nm and Ag(001) with 37 nm. The corresponding rocking curve from the polycrystalline CuTi layer in Fig. 1(c) shows a FWHM of 1.7°. This confirms the strong 001 texture of the CuTi layer deposited on SiO2/Si(001).

Fig. 1(d) is a typical XRD reciprocal space map from the CuTi(001)/MgO(001) layer, showing asymmetric CuTi 204 and MgO 113 reflections using colored iso-intensity contours on a logarithmic scale. The map is plotted in k-space where the in-plane and out-of-plane reciprocal lattice vectors \( k_x \) and \( k_z \) are defined by \( k_x = 2\sin\theta \sin(\omega-\theta) / \lambda \) and \( k_z = 2\sin\theta \cos(\omega-\theta) / \lambda \), respectively. The MgO 113 peak is at \( k_x = 3.322 \pm 0.003 \) nm\(^{-1}\) and \( k_z = 7.132 \pm 0.006 \) nm\(^{-1}\), consistent with a substrate lattice constant of 4.212 Å. The CuTi 204 peak at \( k_x = 6.383 \pm 0.020 \) nm\(^{-1}\) and \( k_z = 6.758 \pm 0.011 \) nm\(^{-1}\) shows broadening along \( \omega \) which is attributed to the mosaic spread representing the misalignment of single crystal blocks within the epitaxial CuTi(001) layers. The peak position provides values for the in-plane and out-of-plane lattice constants \( a = 2/k_x = 3.133 \pm 0.009 \) Å and \( c = 4/k_z = 5.919 \pm 0.010 \) Å. The measured in-plane value is 0.8% larger than the reported \( a = 3.107 \) Å while the measured out-of-
The plane lattice constant matches the reported $c = 5.919 \text{Å}^{35}$ but is 0.4% smaller than the value from the symmetric scan in Fig. 1(a). These deviations can be attributed to experimental uncertainties but suggest also slightly larger relaxed lattice constants for our layers in comparison to the previously reported values and a possible slight biaxial tensile stress due to a mismatch in the thermal expansion coefficients of the substrate and layer.

Fig. 1(e) shows two azimuthal XRD $\varphi$-scans from the same CuTi(001)/MgO(001) sample. The first pattern is obtained with a $\chi = 43.39^\circ$ sample tilt and a fixed $2\theta = 41.87^\circ$ to detect CuTi 102 reflections while the second scan uses $\chi = 25.24^\circ$ and $2\theta = 74.69^\circ$ yielding MgO 113 reflections. Both patterns show four reflections at $\varphi = 45^\circ$, 135°, 225°, and 315°, indicating an in-plane epitaxial relationship where CuTi[100] || MgO[110].

XRD analyses were performed for all samples presented in this study. They exhibit similar results as those shown in Fig. 1, confirming that all CuTi layers deposited on MgO(001) are epitaxial single crystals with CuTi[001] || MgO[001] and CuTi[100] || MgO[110], while all layers deposited on SiO2/Si(001) exhibit a 001-textured polycrystalline microstructure.

Fig. 2(a) shows a typical XRR result from a 33.3-nm-thick epitaxial CuTi(001)/MgO(001) layer. The measured intensity is plotted as brown curve while the result from curve fitting is depicted as green line, offset by a factor of 10 for clarity purposes. The characteristic interference fringes vs scattering angle $2\theta$ are well described by the curve fitting which provides values for the thickness of the CuTi layer as well as a surface oxide of 33.3 and 2.1 nm, respectively. We note that some of the deposited CuTi is consumed by the growing surface oxide such that the ex situ measured CuTi thickness is smaller than the in situ as-deposited thickness. To quantify this effect, we assume that a stoichiometric Cu:Ti = 1:1 ratio is retained during surface oxidation and approximate the oxide as a mixture of CuO and TiO2. Using the known densities for CuO$^{52}$ and TiO2$^{53}$ we determine that the measured oxide thickness $d_{ox} = 2.1$ nm corresponds to the consumption of 1.2 nm pristine CuTi, yielding a value for the as-deposited thickness prior to air exposure of 34.5 nm. This value is slightly smaller than the expected 38.0 nm from the deposition rate. The XRR analysis also provides values for the root-mean-square (RMS) surface roughness $\sigma = 3.0$ nm. Similar XRR measurements are performed for all CuTi films with $d < 100$ nm, indicating 2.1-3.1 nm thick surface oxides and yielding ex situ measured thicknesses $d = 5.8 - 73.2$ nm and corresponding as-deposited in situ $d = 7.3 - 74.9$ nm, as listed in Table I. The as-deposited thickness $d_a = 151$ nm for the thickest layer is determined from the deposition rate, while the ex situ thickness $d = 149$ nm is estimated assuming a 2-3 nm thick surface oxide, as measured for the thinner layers.

Figures 2(b) and (c) are representative $2 \times 2 \mu m^2$ AFM micrographs from two epitaxial CuTi(001)/MgO(001) layers. They are sections of larger $5 \times 5 \mu m^2$ images that are used for quantitative roughness analyses. The surface morphology of the 21.1 nm thick layer in Fig. 2(b) exhibits $34 \pm 2 \mu m^2$ circular surface mounds with an average width of 120 nm and a peak-to-valley height of 6 nm, yielding a surface roughness $\sigma =$
1.6 nm. In contrast, the 73.2 nm thick layer in Fig. 2(c) shows surface features which suggest coalescence of approximately circular 150-nm-wide mounds into non-uniform shapes with widths ranging from 200 nm to 1 μm, yielding a roughness of 3.2 nm. This suggests that above a critical thickness which allows for full coverage and continuous growth of CuTi on the MgO, the surface roughness originates from the inhomogeneous nuclei growth and coalescence. We note that the surface oxide thickness is small in comparison to the surface morphological features and therefore expect a negligible effect of the surface oxidation on the AFM images. Thus, micrographs are expected to reflect the morphology of the as-deposited CuTi.

Figure 2(d) summarizes the results from the roughness analyses. It is a plot of $\sigma$ vs layer thickness $d$, as determined from both AFM and XRR measurements. Both data sets indicate an increasing $\sigma$ with increasing $d$. More specifically, the roughness is small, $\sigma < 1$ nm, for the thinnest $d = 5.8$ nm layer and continuously increases to reach $\sigma = 3.7$ for $d = 149$ nm. Such an increase in $\sigma$ with increasing $d$ is common during thin film deposition and is attributed to various roughening mechanisms including nuclei formation and kinetic roughening, and is described using power law scaling models.54-57 We note that there is some quantitative variation in the roughness values determined by AFM and XRR as shown in Fig. 2(d). This is attributed to experimental and data-analysis artifacts. More specifically, the depth of a depression or valley measured by AFM is underestimated due to the finite tip radius,58 while the XRR roughness is affected by the substrate roughness, with an average $\sigma = 1.1$ nm for the five samples investigated by XRR. This substrate roughness has large lateral length scales that are not detected by AFM15 and are expected to have a negligible impact on the electron transport discussed below.

Figure 3(a) shows XPS depth profile compositional data from a 33.3-nm-thick CuTi(001)/MgO(001) layer. It is obtained from high-resolution Ti 2p, Cu 2p, Mg 1s and O 1s spectra acquired after each 15 s Ar+ sputter etching step. The plot shows the measured atomic percentage of the selected elements versus sputter depth, indicating a constant (within experimental noise) Cu and Ti content within the layer, with an average atomic composition of 52 % Ti and 48 % Cu, in good agreement with the expected 50:50 ratio for stoichiometric CuTi. This is followed by a sharp transition at a sputter depth of 34.5 nm where the Cu and Ti content drop to zero while the Mg and O content rise each to 50%. The steep transition indicates a sharp layer-substrate interface without any detectable oxidation of the metal nor any detectable Cu or Ti diffusion into the MgO substrate. The initial spectrum prior to sputter etching (0 nm sputter depth) indicates 49 % of oxygen which is ascribed to surface oxidation and adsorbed water. The inset displays Ti 2p core level spectra taken at 0, 2.3, and 4.6 nm sputter depth. The spectrum before sputtering (0 nm) shows the Ti 2p$_{3/2}$ and Ti 2p$_{1/2}$ doublet peaks at 458.8 and 464.4 eV, respectively, close to the reported energies for fully oxidized Ti(IV) of 458.6 and 464.3 eV.59 However, these peaks shift to 454.1 and 460.1 eV after the first cycle of sputter etching (2.3 nm), consistent with metallic Ti(0) with reported energies of 454.0 and 460.0 eV.60 This confirms that the oxidation of the CuTi layer is limited to the surface. In contrast, the measured binding energy of the Cu 2p core level (not shown)
exhibits no detectable shift near the surface. This can be ascribed to either (i) negligible Cu surface oxidation due to the smaller affinity of Cu to oxygen which results in Ti oxidation prior to Cu oxidation or (ii) a low Cu oxidation state at the surface, more specifically Cu(I) since Cu$_2$O has within experimental uncertainty the same Cu 2$p$ binding energy as metallic Cu.

Figure 3(b) shows a typical RBS spectrum from the same 33.3-nm-thick CuTi(001) layer. The measured intensity of backscattered He$^+$ particles vs their energy is plotted as brown star data points while the green curve is the result from curve fitting using the SIMNRA simulation software. The spectrum reveals peaks at $E = 1.41$ MeV and $1.53$ MeV, attributed to Rutherford backscattering at Ti and Cu atoms, respectively. The shoulders at 0.99 and 0.65 MeV represent the onset of backscattering events at Mg and O atoms on the substrate surface. A small intensity variation centered at 0.71 MeV is attributed to oxygen at the CuTi layer surface, confirming the formation of a surface oxide after air exposure detected by XPS and quantified by XRR. The simulated curve describes the measured data well. It is obtained using a three-layer model consisting of a surface oxygen layer, a homogeneous Cu-Ti layer with variable composition and thickness, and a semi-infinite MgO substrate with a fixed 50-50 composition. The fitting procedure yields the atomic areal density of Cu and Ti atoms of $(1.40 \pm 0.05)$ and $(1.31 \pm 0.04) \times 10^{17}$ atoms/cm$^2$, respectively, suggesting a $(52 \pm 2)$ % Cu and $(48 \pm 2)$ % Ti composition which is in good agreement with the XPS results. The measured atomic areal densities correspond to a defect-free CuTi layer with a thickness of 38.7 nm. However, the peak at 0.71 MeV also suggests $(1.83 \pm 0.22) \times 10^{16}$ oxygen atoms/cm$^2$ which form a surface oxide and reduce the effective metallic CuTi thickness. We estimate an oxide thickness of $3.2 \pm 0.4$ nm, assuming stoichiometric oxidation. These thickness values from RBS are in reasonable agreement with the layer and oxide thicknesses of 33.3 and 2.1 nm determined by XRR. In summary, the combination of XPS and RBS analyses indicates that the deposited CuTi layers are homogeneous and stoichiometric. They exhibit a surface oxide and a sharp interface with the substrate.

Figures 4(a) and 4(b) show plots of the calculated CuTi Fermi surface, color coded according to the Fermi velocity $v_f$ and the electron-phonon scattering mean free path $\lambda$, respectively. They are obtained from first-principles density functional calculations as described in the Section II. The tetragonal Brillouin zone is wider within the basal plane than along the z-axis, because the lattice constant $a = 3.09$ Å is smaller than $c = 5.83$ Å. The CuTi Fermi surface is composed of two surfaces which correspond to the two bands that cross the Fermi level. The coloring in Fig. 4(a) indicates a large variation in the Fermi velocity. It is smallest, $v_f = 0.7 \times 10^5$ m/s, approximately halfway between the zone center and the $M$-point along the [110] direction, as indicated by the blue color. In contrast, it is nearly an order of magnitude larger, $v_f = 6.6 \times 10^5$ m/s, along the inner surface. The velocity distribution has a standard deviation of $1.1 \times 10^5$ m/s. We wannierize the electronic energies and corresponding velocities and directly compute the Brillouin zone integral on a finer mesh of $4096 \times 4096 \times 4096$. This numerical integration yields a calculated $\rho_{o\lambda} = 9.56 \times 10^{-16}$ Ω m$^2$ for transport in the basal plane. The corresponding value along the z-direction $\rho_{o\lambda} = 14.91 \times 10^{-16}$ Ω m$^2$ is
1.6 times larger. We note that these values are from pure bulk calculations. In contrast, in the case of a thin film or a wire, the anisotropy in the Fermi velocity can result in an anisotropic resistivity size effect even for cubic materials which exhibit isotropic bulk resistivity.\(^{16,25}\) This is because, for example, a particularly large Fermi velocity perpendicular to the scattering surface results in a larger scattering rate and correspondingly enhanced resistivity size effect. We have recently demonstrated this effect for a large set of materials systems and introduced resistivity scaling coefficients \(r_{\text{film}}\) for thin films and \(r_{\text{wire}}\) for square wires.\(^{25}\) We compute \(r_{\text{film}} = 9.14 \times 10^{-16} \, \Omega \, \text{m}^2\) for a CuTi thin film with an 001 orientation, that is, with (001) terminating surfaces as investigated experimentally. We also compute \(r_{\text{wire}} = 10.17 \times 10^{-16} \, \Omega \, \text{m}^2\) for a CuTi square wire along the in-plane [100] direction. These values are close to the in-plane \(\rho_{\parallel} = 9.56 \times 10^{-16} \, \Omega \, \text{m}^2\) presented above, indicating that accounting for the out-of-plane Fermi velocity component has only a minor effect on the CuTi(001) resistivity size effect. This is attributed to a CuTi Fermi velocity distribution that is not disproportionately concentrated in any one direction despite that the Fermi surface exhibits a considerable anisotropy.

Figure 4(b) is a plot of the same CuTi Fermi surface, color coded according to the electron-phonon scattering mean free path. The distribution of the \(k\)-dependent electron mean free paths is very non-uniform, with values ranging from 0.8 to 8.5 nm, an average \(\lambda = 4.6\) nm and a standard deviation of 1.5 nm. The mean free paths are directly determined from the calculated electron-phonon scattering rates using Fermi’s golden rule. For this, we use the DFT-computed electronic energies, velocities, and electron-phonon matrix elements in the Wannier representation. Subsequently, the resistivities are obtained using the Boltzmann transport equation in the per-band relaxation time approximation. This yields room temperature bulk resistivities \(\rho_{\parallel} = 20.6\) \(\mu\Omega\) cm and \(\rho_{\perp} = 31.0\) \(\mu\Omega\) cm in the basal plane and z-axis, respectively, and corresponding \(\rho_{\parallel,77K} = 2.4\) \(\mu\Omega\) cm and \(\rho_{\perp,77K} = 3.6\) \(\mu\Omega\) cm at 77 K.

Figure 5 is a plot of the measured electrical resistivity \(\rho\) as a function of layer thickness \(d\), as also listed in Table I. The plot includes data from both epitaxial CuTi(001)/MgO(001) layers (red squares) and 001-textured polycrystalline CuTi/SiO\(_2\)/Si layers (blue triangles) measured \textit{in situ} in vacuum at 295 K (solid symbols) and immersed in liquid N\(_2\) at 77 K (open symbols), while the plus symbols are for room temperature \textit{ex situ} measurements after air exposure. The \textit{in situ} room temperature resistivity increases from 19.4 \(\mu\Omega\) cm for the thickest CuTi(001)/MgO(001) layer (151 nm) to 30.3 \(\mu\Omega\) cm for \(d = 7.3\) nm. This 57% resistivity increase is attributed to increasing electron scattering at the CuTi surface and the CuTi-MgO interface with decreasing \(d\), as quantified in Section IV. The \textit{ex situ} values show a 7 – 15 % higher resistivity than measured prior to air exposure. We note that this increase is not simply due to a reduced conductor thickness caused by surface oxidation. In fact, the plotted data points already account for the smaller \textit{ex situ} vs as deposited thicknesses, as quantified with our XRR analyses discussed above. Therefore, we attribute the resistivity increase during air exposure to an increase in diffuse surface scattering, similar to what has previously been reported for Cu,\(^{61}\) Co,\(^{17}\) Nb,\(^{21}\) Ag,\(^{19}\) and Ni,\(^{20}\) and
has been attributed to surface charge transfer which is particularly pronounced for metals with a low electronegativity.\textsuperscript{62} The red open squares in Fig. 5 from the measurements at 77 K show lower $\rho$ values than at room temperature, due to the reduced electron-phonon scattering. The absolute value of this reduction is approximately independent of $d$, indicating that the resistivity contributions from phonon and surface scattering are additive, consistent with Matthiessen’s rule. We note, however, that the relative resistivity size effect is much more pronounced at low temperature, with a 472% increase at 77 K but only a 57% increase at 295 K. This is due to the longer electron mean free path at cryogenic temperatures, as quantified in more detail in Section IV.

The blue symbols in Fig. 5 from the polycrystalline CuTi/SiO$_2$/Si layers indicate a considerably higher resistivity and a more pronounced resistivity size effect than for the epitaxial layers. More specifically, the in situ room-temperature resistivity (blue solid triangles) increases from $\rho = 33.8 \pm 0.5 \, \mu\Omega \, \text{cm}$ for $d = 91.2 \, \text{nm}$ to $\rho = 79.6 \pm 2.9 \, \mu\Omega \, \text{cm}$ for $d = 8.2 \, \text{nm}$. These values are 1.7-2.6 times larger than for epitaxial CuTi(001) with comparable thicknesses, indicating a large resistivity contribution from grain boundary scattering in the CuTi/SiO$_2$/Si layers. The plus symbols from the ex situ data indicate a 3 - 14 $\mu\Omega \, \text{cm}$ resistivity increase upon air exposure. This increase is more pronounced than for epitaxial CuTi(001), which may be ascribed to accelerated or less uniform surface oxidation in the presence of grain boundaries caused by a higher density of surface steps or boundary defect sites which act as oxidation nucleation sites. This is also supported by the fact that the roughness of polycrystalline CuTi films determined by XRR is 0.6, 1.8, 2.6, 3.4, 3.9 nm for $d = 8.2, 15.3, 30.3, 46.1, 91.2 \, \text{nm}$, which is $\sim$20% larger than for the epitaxial layers. We note that a polycrystalline CuTi layer with a nominal thickness of 5 nm exhibits a very large measured resistivity above 100 $\mu\Omega \, \text{cm}$, similar to recent reports for polycrystalline NiAl\textsuperscript{27,28} and CuAl$_2$.\textsuperscript{29} This large resistivity is attributed to a small grain size and a partially discontinuous microstructure associated with an incomplete nuclei coalescence for $d = 5 \, \text{nm}$, similar to what has been reported for thin Ir\textsuperscript{22} and Rh\textsuperscript{63} layers. The blue open triangles from the measurements at 77 K are approximately 20 $\mu\Omega \, \text{cm}$ below the ex situ room-temperature values for all $d$. This temperature effect is similar to that for the epitaxial layers and suggests approximately additive contributions from electron scattering at phonons, surfaces, and grain boundaries.

IV. DISCUSSION

We now discuss the presented transport data using the classical FS\textsuperscript{9,10} and MS\textsuperscript{11} models for surface and grain boundary scattering. For this purpose, we start with the epitaxial layers since the absence of grain boundaries simplifies data fitting and analysis. Firstly, we assume completely diffuse surface scattering by setting the specularity parameters at both surfaces to zero ($p_1 = p_2 = 0$). This assumption results in a bulk mean free path $\lambda$ which can be understood as an upper bound to possible $\lambda$ values or alternatively as the bulk electron mean free path for the case of completely diffuse surface scattering. This approach is chosen since typical $\rho$ vs $d$ data do not allow to independently determine both $\rho$ and $\lambda$,\textsuperscript{16,21} and has previously been applied to determine
the effective mean free path of Ir,\textsuperscript{22} Rh,\textsuperscript{18} Co,\textsuperscript{17} Ru,\textsuperscript{15} and Ti\textsubscript{4}SiC\textsubscript{3}.\textsuperscript{24} The red solid line in Fig. 5 is obtained from curve fitting to the \textit{in situ} room-temperature data employing the (exact) integral form of the FS model\textsuperscript{6,9,10} and using \( \lambda \) and the bulk resistivity \( \rho_0 \) as free fitting parameters. This yields \( \rho_0 = 19.2 \ \mu\Omega \) cm and \( \lambda = 9.8 \) nm for the \textit{in situ} data. Similar analyses for the low temperature and air exposed resistivities result in \( \rho_0 = 3.3 \ \mu\Omega \) cm and \( \lambda = 68.5 \) nm at 77 K, and \( \rho_0 = 19.8 \ \mu\Omega \) cm and \( \lambda = 12.5 \) nm for the room-temperature \textit{ex situ} data, as also summarized in Table II. We note that \( \rho_0 \) at 77 K is approximately six times smaller than at room temperature, while \( \lambda \) is approximately six times larger. This is attributed to a six times smaller electron phonon scattering at low temperatures and indicates, as expected from classical transport models,\textsuperscript{12} that the \( \rho_0\lambda \) product is temperature independent. This product is a common benchmark quantity to evaluate the resistivity scaling\textsuperscript{12,64} and is \( 24.7 \times 10^{-16} \ \Omega \) m\textsuperscript{2}, as obtained from the \textit{ex situ} measured air exposed CuTi(001) samples.

The room temperature \( \rho_0 = 19.2 \) and 19.8 \( \mu\Omega \) cm measured \textit{in situ} and \textit{ex situ} are nearly identical within experimental uncertainty, yielding an average \( \rho_0 = 19.5 \pm 0.3 \) \( \mu\Omega \) cm. In contrast, the \( \lambda \) values from direct fitting deviate considerably. More specifically, the \textit{in situ} data yields a 22 \% smaller \( \lambda \) than the air exposed samples. This is attributed to partial specular surface scattering at the CuTi-vacuum interface. That is, the initial assumption of \( p_1 = 0 \) at the CuTi(001) surface is not valid for the \textit{in situ} data. Conversely, air exposure causes a transition to diffuse scattering at the oxidized CuTi surface, leading to a resistivity increase during air exposure. We postulate \( p = 0 \) for the air exposed \textit{ex situ} data, similar to what has previously been reported for other metals including Cu\textsuperscript{65} and Co\textsuperscript{17} where air exposure results in a transition from partial specular to completely diffuse surface scattering.\textsuperscript{15,66} The \( p = 0 \) assumption for air exposed samples is supported by resistivity measurements as a function of air exposure time. More specifically, the surface oxidation is expected to cause a decrease in the surface scattering specularity until \( p = 0 \) is reached. However, the resistivity measured after 1 min and after two days of air exposure of CuTi(001) surfaces is identical, indicating no change in surface scattering specularity despite the continued growth of the surface oxide, suggesting that \( p = 0 \) is already reached for all \textit{ex situ} measurements both at 295 and 77 K. Following these arguments, the above data fitting with \( p = 0 \) yields the correct room temperature \( \lambda = 12.5 \) nm from the \textit{ex situ} data, while the effective \( \lambda = 9.8 \) nm from the \textit{in situ} data is an underestimation. Thus, in a second step, we fix \( \lambda = 12.5 \) nm and use \( p_1 \) as a new free fitting parameter to describe the \textit{in situ} data, assuming that the electron scattering at the bottom interface (CuTi/MgO) remains completely diffuse (\( p_2 = 0 \)) which is attributed to local epitaxial strain fields and asymmetric covalent bonding that leads to potential perturbation and localized interface states.\textsuperscript{5,37} This yields \( p_1 = 0.5 \) for the \textit{in situ} room-temperature data. That is, both the \textit{in situ} and \textit{ex situ} room temperature resistivity is well-described using a constant \( \lambda = 12.5 \) nm and a constant scattering specularity \( p_2 = 0 \) at the bottom surface, but a top surface specularity that decreases from \( p_1 = 0.5 \) in vacuum to \( p_1 = 0 \) after air exposure.

We now directly compare the measured size-dependent resistivity data with our first-principles transport predictions. The calculated room temperature bulk resistivity
is 20.6 $\mu$Ω cm in the basal plane, in excellent agreement with the experimental average $\rho_o = 19.5$ $\mu$Ω cm. There is also reasonable agreement in the resistivity at 77 K, with 2.4 and 3.3 $\mu$Ω cm from first-principles predications and measurements, respectively. That is, calculations and experiments agree within ~ 1 $\mu$Ω cm at both temperatures, corresponding to a 5 % and 27% relative deviation. The larger relative deviation at 77 K is attributed to the smaller electron-phonon scattering rate at low temperatures, such that the resistivity contribution from defect scattering in the measured CuTi(001) layers is more pronounced. Nevertheless, there is overall excellent agreement between experiment and simulations for the CuTi bulk resistivity. In contrast, predictions and measurements of the $\rho_o \lambda$ product deviate considerably. More specifically, the predicted $\rho_o \lambda$ values for the basal plane in CuTi are $9.56 \times 10^{-16}$ and $9.14 \times 10^{-16}$ Ω m² for bulk CuTi and CuTi(001) thin films, respectively, while the measured effective $\rho_o \lambda = 24.7 \times 10^{-16}$ Ω m². That is, the experimental resistivity size effect is more than a factor of two larger than predicted from first principles, as also evident for the effective $\lambda$ values listed in Table II. A similar deviation with a resistivity size effect that is larger from experiment than predicted from the bulk electronic structure and the FS model has been previously reported for a range of metals including W,16 Nb,21 Ni,67 and CuAl2.30 There are various physical reasons which may cause this deviation: (1) The measured CuTi residual resistivity at 77 K is more than 3 $\mu$Ω cm, suggesting a considerable resistivity contribution from electron scattering at crystalline defects including vacancies, impurities, anti-site substitutions and dislocations. If the point-defects and/or misfit dislocations have a more pronounced effect on the resistivity for thinner layers, the measured resistivity size effect and, in turn, the measured effective mean free path is artificially exacerbated. This argument is particularly plausible for the strain field of misfit dislocations at the MgO-CuTi interface which are expected to only affect the resistivity near the substrate-layer interface. (2) The surface roughness of the thin samples represents a larger fraction of the overall layer thickness and may therefore cause a more pronounced resistivity roughness effect.68 Conventional classical transport models indicate that the largest possible resistivity contribution from surface roughness corresponds to diffuse surface scattering ($p = 0$) in combination with a geometric correction.69 However, more recent results suggest that the roughness effect can be stronger, resulting in an apparent (unphysical) $p < 0$.66,68 (3) The semiclassical FS model which is used in combination with the first-principles predictions may underestimate the resistivity size effect in the limit of narrow conductors. This is because the FS model considers the electron as a point particle which exhibits classical scattering events. Correspondingly, this model has no explicit relaxation associated with electron-surface interactions, leading to diverging (incorrect) resistivity predictions in the limit of thin wires and low temperatures (i.e. for large $\lambda/d$ ratios).8,70,71

We now discuss the resistivity of the polycrystalline CuTi/SiO2/Si layers. They exhibit a higher $\rho$ than the epitaxial layers which is attributed to electron scattering at grain boundaries. This effect is most commonly described using the MS model for grain boundary scattering which predicts the resistivity contribution using two parameters: the boundary reflectivity $R$ and the average grain size $D$.11 The blue solid curve through
the square data points in Fig. 5 are obtained from curve fitting to the \textit{in situ} measured resistivity, using a combined FS and MS model.\(^6\) However, to limit the number of free parameters during the fitting procedure, we keep \(\rho_0 = 19.5 \ \mu\Omega \text{ cm} \) and \(\lambda = 12.5 \ \text{nm} \) fixed at the values obtained from data fitting of the epitaxial layers. This effectively means that we regard the difference between the resistivity of polycrystalline and epitaxial CuTi layers as the electron grain boundary scattering contribution and neglect the influence of possible differences in crystallographic defects. This approximation is justified by the similarity of the two sample sets, particularly the same deposition temperature of 350 °C (causing a comparable expected point-defect concentration) as well as the same 001 out-of-plane crystalline orientation (causing the same (001) facets for electron surface scattering). We note that the remaining two parameters \(R\) and \(D\) cannot be independently determined from the measured resistivity and, in addition, \(D\) is expected to be a function of \(d\) and even increases with height within a single layer. Correspondingly, we continue the data analysis by assuming a fixed \(R\) to determine an effective \(D\) vs \(d\) relationship. Previous work on grain boundary scattering found that \(R\) is a function of both the conductor materials and the grain orientation distribution. Many reported values for \(R\) are within the range 0.4 - 0.6.\(^6,18,32,63,72-74\) Thus, as an estimate, we semi-arbitrarily fix \(R = 0.5 \pm 0.1\) for CuTi and employ the approximate expression from the combined FS+MS model:\(^6,8\)

\[
\rho = \rho_0 + 3\rho_0 \lambda (1 - p) / 8d + 3R\rho_0 \lambda / 2D(1 - R)
\]

(1)
to determine the grain size for each thickness. For example, the measured room-temperature resistivity of the thickest CuTi layer \((d = 91.2 \ \text{nm})\) yields \(D = 17.6, 26.4, 39.6 \ \text{nm}\) for \(R = 0.4, 0.5, 0.6\), respectively. Corresponding data analyses of the \textit{in situ} resistivity for all layers indicates that the effective grain size increases with thickness, with \(D = 7.2 \pm 3.6, 12.4 \pm 6.2, 15.6 \pm 7.8, 20.7 \pm 10.3, \) and \(26.4 \pm 13.2 \ \text{nm}\) for \(d = 8.2, 15.3, 30.3, 46.1 \) and 91.2 nm. That is, there is a nearly linear correlation between grain size and thickness, with \(D = 0.21 \ d + d_0\) where \(d_0 = 8.6 \ \text{nm}\). This expression, together with the FS+MS model, yield the blue solid line in Fig. 5. The same expression for the grain size is also used to determine the dashed blue line for the resistivity data at 77 K. This is done without any new fitting parameters such that the dashed blue curve in Fig. 5 is the direct result from the bulk resistivity from the epitaxial layers and the room temperature grain size analysis. This curve agrees very well with the measured \(\rho\) at 77 K, confirming that the grain size distribution and the electron grain boundary reflection probability are temperature independent, as expected from classical transport models. That is, the good agreement supports the chosen approach for data analysis and interpretation.

V. CONCLUSIONS

CuTi layers that are deposited at 350 °C on MgO(001) substrates form epitaxial stoichiometric layers, as confirmed by XRD, XPS and RBS analyses. \textit{In situ} and \textit{ex situ} transport measurements show a resistivity size effect that is well described with the classical FS model and an effective room-temperature bulk electron mean free path \(\lambda = 12.5 \pm 0.6 \ \text{nm}\) and bulk resistivity \(\rho_0 = 19.5 \pm 0.3 \ \mu\Omega \text{ cm}\). Air exposure causes a
transition from partially specular surface scattering with \( p = 0.5 \) for the as-deposited layers to completely diffuse surface scattering with \( p = 0 \). First-principles calculations yield \( \rho_0\lambda = 9.6 \times 10^{-16} \Omega \text{m}^2 \) in the basal plane. This is 61% smaller than the experimental \( \rho_0\lambda = 24.7 \times 10^{-16} \Omega \text{m}^2 \). The large deviation may be attributed to surface roughness, thickness-dependent crystallographic defects and/or the breakdown of the semiclassical transport model in the limit of narrow conductors. Polycrystalline CuTi layers deposited on SiO₂/Si substrates have a 74 - 163 % larger room-temperature resistivity. This is attributed to electron scattering at grain boundaries with an effective grain size that increases with from \( 7.2 \pm 3.6 \) nm for \( d = 8.2 \pm 0.3 \) nm to \( 26.4 \pm 13.2 \) for \( d = 91.2 \pm 1.3 \) nm. The overall results suggest that the CuTi compound has no intrinsic conduction benefit at small dimensions in comparison to elemental metals like Cu and Co. However, the expected larger stability of CuTi in comparison to Cu in direct contact with SiO₂ may provide reliability benefits and a liner thickness reduction, with the potential for a superior conductance of narrow CuTi interconnect lines.

Acknowledgments
The authors acknowledge funding from the Semiconductor Research Corporation under tasks 2966.003 and 2966.002, and the NY State Empire State Development's Division of Science, Technology and Innovation (NYSTAR) through Focus Center-NY–RPI Contract C180117.

Data availability
The data that support the findings of this study are available within this article. Some additional data related to the first-principles simulations are available from the authors upon reasonable request.

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https://doi.org/10.1063/5.0135132

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Figures

Fig. 1. Representative (a) \( \theta-2\theta \) scans, (b,c) \( \omega \) rocking curves from the CuTi 001 reflection, (d) reciprocal space map and (e) \( \varphi \)-scan of CuTi 102 and MgO 113, from a 33.3-nm-thick epitaxial CuTi(001)/MgO(001) layer (red) and a 44.3-nm-thick polycrystalline CuTi layer on SiO\(_2\)/Si(001) (blue).
Fig. 2. (a) XRR scan including result from curve fitting from a $d = 33.3$ nm thick CuTi layer, (b) and (c) representative AFM images for $d = 21.1$ and $73.2$ nm, and (d) RMS surface roughness $\sigma$ vs $d$ as measured by XRR and AFM, from epitaxial CuTi(001)/MgO(001) layers.
Fig. 3. Representative (a) XPS depth profile and (b) RBS spectrum from a 33.3-nm-thick CuTi(001)/MgO(001) layer. The inset in (a) shows the Ti 2p peaks vs binding energy (B.E.) at the surface prior to sputter etching (0 nm) and at a sputter depth of 2.3 and 4.6 nm.
Fig. 4. Fermi surface of CuTi color coded according to (a) the Fermi velocity $v_F$ and (b) the electron mean free path $\lambda$. 
Fig. 5. Resistivity $\rho$ vs layer thickness $d$ of epitaxial CuTi(001)/MgO(001) (red) and polycrystalline CuTi/SiO$_2$/Si (blue) layers measured in situ (solid symbols) and ex situ (plus symbols) in vacuum and air at 295 K, respectively, and immersed in liquid N$_2$ at 77 K (open symbols). Curves are from data fitting using the FS and MS models.
https://doi.org/10.1063/5.0135132

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Table I. Measured layer thickness $d_m$, surface oxide thickness $d_{ox}$, as-deposited thickness $d_a$ prior to air exposure, and resistivity $\rho$ measured in situ in vacuum and ex situ after air exposure at 295 K, and immersed in liquid N$_2$ at 77 K, from epitaxial CuTi(001)/MgO(001) and polycrystalline CuTi/SiO$_2$/Si layers.
Table II. Bulk resistivity $\rho_0$ and effective bulk mean free path $\lambda$ for CuTi, measured \textit{in situ} and \textit{ex situ} at 295 K and immersed in liquid N\textsubscript{2} at 77 K, and simulated by first-principles calculations for in-plane and $z$-axis transport directions at 298 and 77 K, and thin film and wire geometries at 298 K.