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# Measuring the Mean Inner Potential Of $Al_2O_3$ Sapphire Using Off-axis Electron Holography

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The mean inner potential (MIP, $V_0$) of solids is the volume averaged electrostatic (Coulomb) potential between the material and vacuum, thus sensitive to charge-density distributions related to the chemical bonding of a crystal [1]. Here, we measure the MIP of α-$Al_2O_3$ sapphire (corundum) using off-axis electron holography. We used wedge specimens for the transmission electron microscope, mechanically polished at an angle of approximately 45° with respect to the (0001) basal plane. The angle of the wedge sample is determined by confocal optical microscopy and by direct observation in the TEM following subsequent perpendicular focused ion beam sectioning of the samples, e.g. Fig. 1. An example of a reconstructed electron phase map from such a wedge sample is shown in Fig. 2. This wedge sample can improve the accuracy of the MIP measurement due to gradients of phase variations, $\Delta\phi$, of the reconstructed electron-wave which originate only from the crystal sample. Therefore, the MIP can be determined according to Eq. (1), assuming the absence of charge distribution and dynamical diffraction.

(1) $V_0=(1/C_E)\cdot(d\Delta\phi/dx)/(dt/dx)$

Where $x$ is the in-plane sample coordinates, $t$ is the sample thickness, and $C_E$ is the interaction constant.

Our measurements [2] concluded that the MIP of sapphire for this geometry is $16.90 \pm 0.36$ V. This measurement indicates that chemical bonding in sapphire is mostly ionic to a degree of 66% ± 8% based on comparisons to weighted electron atomic scattering factors of ions and neutral atoms [3]. However, comparing the MIP with scattering properties of isolated atoms cannot account correctly for chemical bonding in the crystal and ignores the role of crystallographic surfaces. So, we compared these measurements to density-functional-theory calculations based on VASP. We implemented a computationally fast projector augmented wave based plane-wave code to calculate the MIP of a crystal using a straightforward method that can be applied easily and efficiently to any slab. Calculations of α-$Al_2O_3$ slabs cut along (0001) and (1-100) planes indeed show significant differences for MIP values of 15.7 V and 16.7 V, respectively. Finally, the plasmon mean free path for inelastic scattering (IMFP) can also be extracted from this wedge sample, at an improved accuracy, by applying the log-ratio method to zero-loss and energetically unfiltered TEM images. The IMFP of sapphire was measured at 136±2 nm for electrons with 200keV kinetic energy and a semi collection angle of $\beta$=18 mrad.

We will present applications of this wedge approach to measure the MIP of additional crystals: hematite and graphite.

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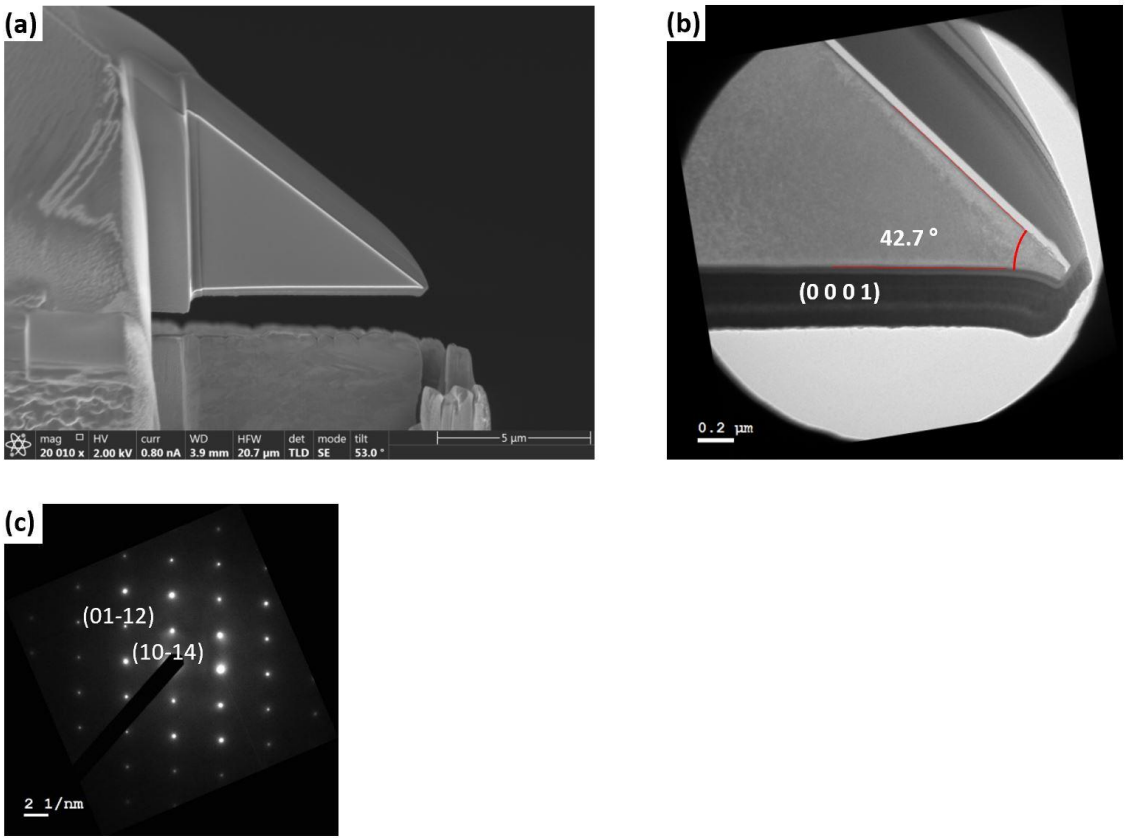


**Figure 1.** α-Al2O3 wedge TEM sample: (a) Secondary electron SEM micrograph of the FIB cross-sectioned sample (b) Bright field cross- sectional TEM micrograph of the wedge sample from which the angle is measured (d) SAED pattern recorded from (b) showing a zone axis of [2-1-10], which is an edge-on view on the basal plane.

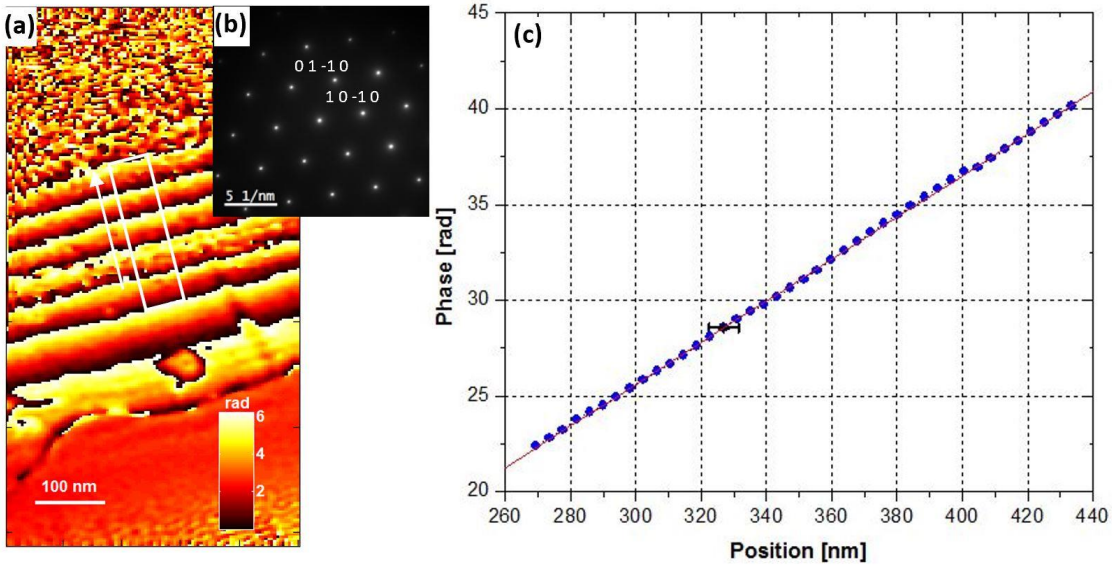


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**Figure 2.** (a) Reconstructed electron phase map (wrapped) from a sapphire wedge sample (b) SAED pattern from [0001] zone axis of α-Al2O3 sapphire, (c) Unwrapped phase variations as a function of position along the direction denoted schematically by the white rectangle in (a).

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