Factors Affecting Measurements of Semiconductor Mean Inner Potentials

Robert S. Pennington*[1], Jens J. Mortensen[2], Takeshi Kasama[3], Chris Boothroyd[4], Rafal E. Dunin-Borkowski[5]

Introduction

The mean inner potential (MIP) is of interest for electron holography, where it affects the measured phase[1]. But, there is large variation in experimental measurements of the MIP. Therefore, calculations may provide guidance on interpretation of experimental measurements, especially on the role of the surface.

In this work, we use density functional theory to calculate mean inner potentials of semiconductors. The stability of the simulator with respect to calculation parameters is found. These conditions are then used to simulate the mean inner potential for silicon under different surface conditions, including surface facet, adsorbates, and surface reconstruction. The effect of diffraction contrast on phase profiles of nanowires is also examined experimentally.

Density Functional Theory and GPAW

Density functional theory (DFT) allows for the calculation of electronic structure. The grid-based projector-augmented wave method, implemented as the GPAW simulator by CAMD at DTU, allows for real-space calculation of the electron density[2]. This allows for convenient mean inner potential calculations.

Calculation Geometry

**Objective:** Use calculation geometry that allows MIP calculations.

The MIP calculation requires the potential in a region of vacuum, labeled A, to be compared to the potential in a region of material, labeled B. With the [100] direction normal to the surface, the surfaces of zincblende compound semiconductor slabs are nonpolar. This is the same calculation geometry used elsewhere [3].

Verification of Simulator

**Objective:** Verify that calculations of the MIP vary little when calculation parameters are changed.

The MIP was relatively independent of exchange-correlation functional. The PBE functional was used as standard.

Calculated Mean Inner Potentials

**Objective:** Calculate MIP material and surface dependence.

Even though the mean inner potential is measured in the middle of the slab relative to vacuum, adsorbate element and position have a measurable effect. Adsorbates were placed as seen below, and allowed to relax. White atoms are S, black atoms are adsorbate.

Electron Holography

**Objective:** Examine how diffraction contrast affects electron holograms.

The chosen surface facet affects the MIP. The difference between [100] surfaces with and without a (2x1) reconstruction is 0.59V, but the differences between other surface facets are smaller [0.05V].

The MIPs calculated here are consistent with literature values for DFT calculations of these materials[3]. The substantial difference between the result from DFT calculation and the results from electron scattering factor[4][5] indicates the importance of electronic structure for MIP calculations.

Conclusions & Further Work

**Conclusions:** We have calculated mean inner potentials of both compound and elemental semiconductors. Surface morphology and composition both affect the mean inner potential in the middle of the slab. Diffraction contrast can affect holograms and, therefore, the mean inner potential measured.

**Further Work:** Further work on calculations of mean inner potential should explore the effects of surface orientation and composition of both stoichiometry and atom positions. Further experimental work should examine ways of determining the mean inner potential of a material with known atom positions.

References:

[1]: Introduction to Electron Holography, edited by Völkl et al. 1999

Line profiles across sections of reconstructed phase images taken at different tilts from zone axis. The nanowire was tilted about its long axis, so the thicknesses and phase changes should be similar; they are not, due to contributions from diffraction contrast.

Mean inner potential measurements would depend strongly on crystallographic orientation.