Strategies for Analyzing Non-Common-Atom Heterovalent Interfaces: The Case of CdTe-on-InSb

E. Luna[1], A. Trampert[1], J. Lu[2], T. Aoki[3], Y.-H. Zhang[4], M.R. McCartney[5], and D. J. Smith[5]

[1] Paul-Drude-Institut für Festkörperelektronik Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, D-10117 Berlin, Germany

[2]School of Engineering for Matter, Transport and Energy, Arizona State University, Tempe, AZ 85287, USA

[3] LeRoy Eyring Center for Solid State Science, Arizona State University, Tempe, AZ 85287, USA

[4] School of Electrical, Computer and Energy Engineering, Arizona State University, Tempe, AZ 85287, USA

[5] Department of Physics, Arizona State University, Tempe, AZ 85287, USA

Semiconductor heterostructures are intrinsic to a wide range of modern-day electronic devices. Knowledge of chemical interfacial profiles in these complex structures is critical to the task of optimizing the device performance. Here, we report on an innovative methodology that enables reliable interface structure analysis of non-common-atom heterovalent interfaces on all relevant length scales from hundred-nm to atomic resolution.

Non-common-atom (NCA) heterovalent interfaces offer potential benefits arising from the valence mismatch but also contain challenges due to the large charge imbalances. Whether a sharp polar interface is formed or, on the contrary, there are mixtures of chemical bonds across the interface leading to a nonpolar graded interface is under intense discussion. Furthermore, very little has so far been done to exploit the opportunities offered by NCA heterovalent interfaces, in part due to challenges determining the structure and properties of these types of interfaces, for example, by using scanning transmission electron microscopy (STEM) techniques. This work presents a comprehensive analysis of the composition profile across the case study NCA heterovalent CdTe/InSb interface, carried out using a combination of (S)TEM imaging and spectroscopic techniques. Techniques such as high-angle annular-dark-field and large-angle bright-field STEM, as well as electron energy-loss spectroscopy, give results from the interface region on the atomic scale. These measurements, however, are inherently difficult to interpret because of the close atomic numbers of the constituent elements. In contrast, use of the 002 dark-field TEM imaging mode emphasizes the interface location by comparing differences in structure factors between the two materials. Based on the 002 dark-field TEM, a methodology was developed for reliable determination of the composition profile across the interface and systematic quantification of the interface width. Since the identities of both cations and anions change across the heterointerface, the respective contributions of different elements need to be inserted separately. The intermixing at each sub-lattice is thus independently and completely determined. Comparisons of experimental and simulated CdTe-on-InSb profiles reveal that the interface is structurally abrupt to within about 1.5 nm defined by the variation between 10 and 90%. The present investigation opens new routes to the systematic investigation of heterovalent interfaces, formed by the combination of other valence-mismatched material system.

[+] Author for correspondence: luna@pdi-berlin.de

Supplementary Pages (Optional)

Coherent, defect-free CdTe/InSb interface probed on different length scales (a) $\mathbf{g}_{002}$ dark-field (DF) TEM micrograph and (b) atomically-resolved aberration-corrected scanning transmission electron microscopy (STEM), resolving projections of individual atomic columns ("dumbbells"). Although aberration-corrected STEM allows polarity determination, the exact CdTe/InSb interface position cannot be determined unambiguously. In contrast, use of the chemically sensitive $\mathbf{g}_{002}$ DFTEM imaging technique emphasizes the interface location as shown in Fig. 1(a) [inset: I_{002}^{exp} intensity line-scan used to evaluate the ratio R_{002}^{exp} ($I_{002}^{CdTe}/I_{002}^{InSb}$)]. Schematic representation of the proposed methodology and, in particular, of the iterative procedure used to determine the composition profiles across the NCA heterovalent CdTe/InSb interface: (c) composition profiles for Cd and Te, each based on sigmoidal functions and independently inserted into the calculation, used as input for the calculation of R_{002} ($I_{002}^{CdTe}/I_{002}^{InSb}$) and (d) comparison made with R_{002}^{exp} until best fit obtained. The method allows investigation of the distribution profile for each element separately. The interface is abrupt to within about 1.5 nm (10–90% criterion).

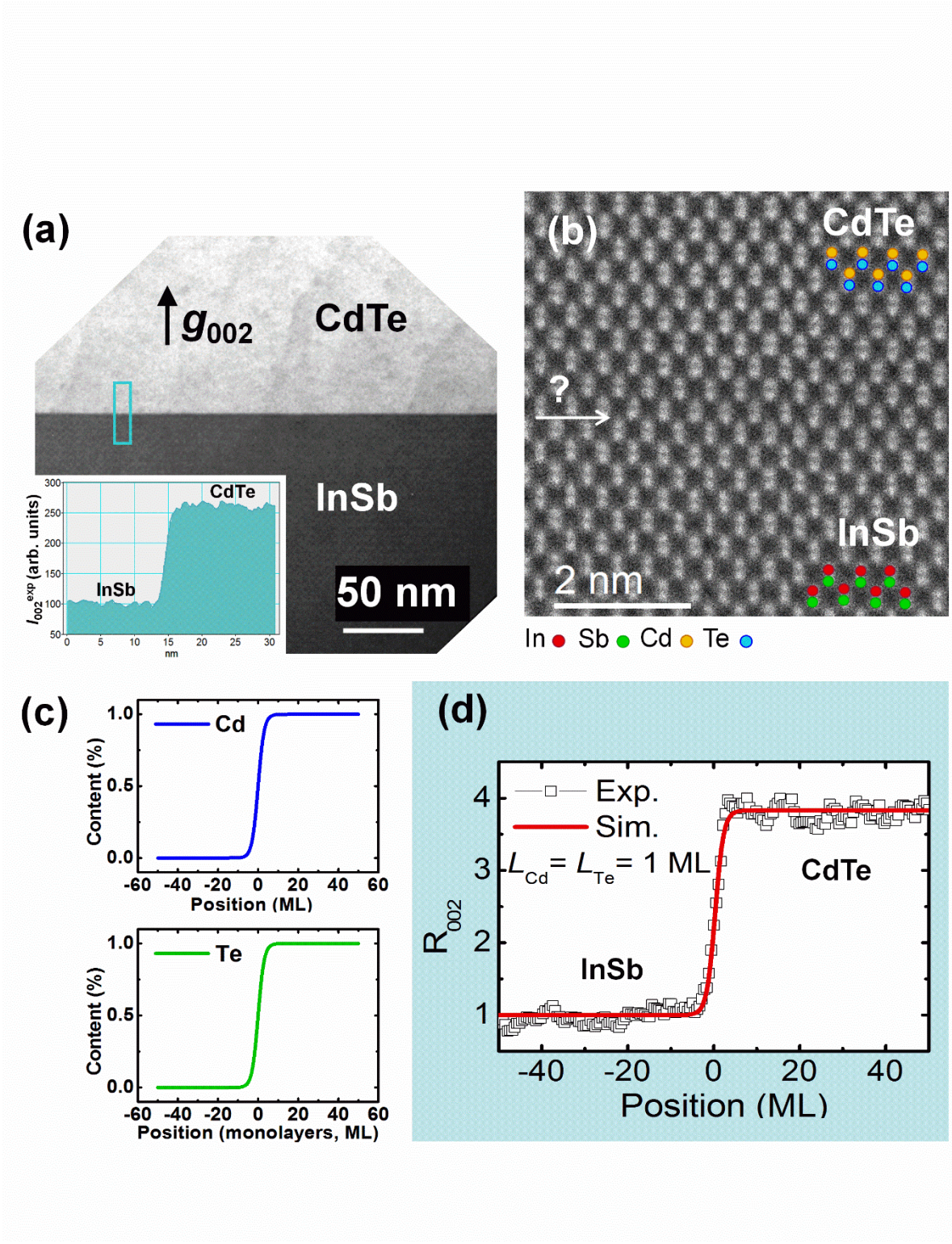
(a)
g_{002}
CdTe
InSb
50 nm
I_{002}^{exp} (arb. units)
nm
(b)
CdTe
InSb
?
2 nm
In Sb Cd Te
(c)
Cd
Content (%)
Position (ML)
Te
Position (monolayers, ML)
(d)
Exp.
Sim.
$L_{Cd} = L_{Te} = 1$ ML
CdTe
InSb
R_{002}
Position (ML)

Figure 1