HL 5 Grenz- und Oberflächen

Zeit: Freitag 10:45–11:45 Raum: TU P-N202

HL 5.1 Fr 10:45 TU P-N202

Simulations of electrical force spectra obtainable on semiconductive surfaces — •F. Müller, A.-D. Müller, and M. Hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, 09107 Chemnitz

The electrical forces between a metallic tip and a semiconductive surface, as detected in Electrical Force Microscopy (EFM), have been studied for various geometries and substrate properties with the finite element simulation tool FEMLab in two and three dimensions. The electrical force components and their second derivative with respect to the bias have been calculated in dependence on the distance and the tip diameter, because this information is directly comparable with electrical force measurements. The lateral resolution achievable with electrical measurements and its dependence on the substrate properties and the tip geometry are derived and explained quantitatively.

HL 5.2 Fr 11:00 TU P-N202

Analyse des strukturellen Übergangs zwischen c-Si/a-Ge: Theorie und Anwendung — •Karsten Thiel[1], Nikolai Borgardt[2], Boris Plikat[3], Tore Niermann[1] und Michael Seibt[1] — [1]IV. Physikalisches Institut der Universität Göttingen und SFB 602, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Moscow Inst. of Electronic Technologie, 124498 Moscow, Russland — [3]Infineon Technologies, Regensburg

Der strukturelle Übergang zwischen amorphen und kristallinen Materialien wird auf der Basis der hochauflösenden Transmissionselektronenmikroskopie (HRTEM) mittels einer Methode, die die Mittelung der Abbildungen entlang der Grenzfläche beinhaltet, am System c-Si/a-Ge untersucht. Diese gemittelten Abbildungen können unter Verwendung einer zweidimensionalen Verteilungsfunktion, die auf der amorphen Seite durch die mittlere atomare Dichte an der Grenze und auf der kristallinen Seite durch die bekannten Positionen der Atome beschrieben wird, mittels konventioneller Multi-Slice-Verfahren simuliert werden.

Neben der theoretischen Beschreibung werden auch Fragen der praktischen Anwendung diskutiert, wie die Frage der lateralen Auflösung dieses Ansatzes sowie die Frage nach signifikanten Unterschieden in den Verteilungsfunktionen unterschiedlicher Abbildungs- bzw. Mittelungsbereiche.

Durch das kontinuierliche Verschieben des Mittelungsbereiches entlang der Grenzfläche und Variation der lateralen Grösse ist es desweiteren möglich, Informationen über den Verlauf des Übergangs entlang dieser Grenze zu erhalten.

[1] N.I. Borgardt et al., Ultramicroscopy **90** (2002), 241.
[2] N.I. Borgardt et al., Phys. Rev. B **70** (2004), 195307.

HL 5.3 Fr 11:15 TU P-N202

Interatomic bond-order potentials for modelling the growth of semiconductor films — •Ralf Drautz[1], Duc Nguyen-Manh[2], Dewey A Murdick[3], Xiaowang Zhou[3], Brian Gillespie[3], Haydn N G Wadley[3], and David G Pettifor[1] — [1]Department of Materials, University of Oxford, Oxford, UK — [2]Theory Modelling Department, Culham Science Centre/UKAEA, Abingdon, UK — [3]School of Engineering and Applied Science, University of Virginia, Charlottesville VA, USA

Interatomic potentials for simulating the growth of semiconductor films must be able to describe bond breaking and remaking naturally within their remit. In this talk we outline the derivation of interatomic bond-order potentials (BOPs) for sp-valent systems by two well defined approximations within density functional theory. The resulting BOPs include a systematic variation of the bond order with band filling as well as environment dependent screening and are therefore applicable to sp-valent systems in general. As an example, we will discuss simulations of the growth of Si thin films.

HL 5.4 Fr 11:30 TU P-N202

Band alignment in $CuIn_5S_8$ / CuI heterostructures — •Igor Konovalov, Liudmila Makhova, and Rüdiger Szargan — Universität Leipzig, Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Linnéstr. 2, 04103 Leipzig

Being a typical n-type semiconductor, $CuIn_5S_8$ spinel has a band gap of 1.5 eV. We studied the valence band alignment at the interface between $CuIn_5S_8$ and the typical p-type transparent semiconductor CuI using X-ray photoelectron spectroscopy. Single crystalline $CuIn_5S_8$ was cleaved in-situ and CuI sublimating from a Knudsen cell at 360 °C resulted in a deposition rate of 0.3 Å/min. The band discontinuity was found to include a minor cliff for the minority holes of about 0.1 eV. In non-epitaxial heterojunctions, band alignment with a cliff generally enhances the interface recombination current mechanism through the junction due to the narrowing of the band gap at the interface for the cross-interface recombination involving the interface states. However, the cliff height found here is significantly smaller than that observed in $AgIn_5S_8$ / CuI heterojunctions before. This trend is in correspondence with the larger band gap of $AgIn_5S_8$ and with the doping pinning rule in its application to sulfidic semiconductors close to the equillibrium.