

HL 40: Impurities / Amorphous Semiconductors

Time: Tuesday 11:30–13:15

Location: EW 015

HL 40.1 Tue 11:30 EW 015

The dangling-bond defect in crystalline and amorphous silicon: insights from ab initio calculations of EPR parameters

— ●GERNOT PFANNER, CHRISTOPH FREYSOLDT, and JÖRG NEUGEBAUER — Max-Planck Institut für Eisenforschung, Max-Planck Strasse 1, D-40237 Düsseldorf

The efficiency of thin-film a-Si:H solar cells is severely limited by light-induced defects (Staebler-Wronski effect). In this context, electron-paramagnetic resonance (EPR) is a key technique to probe for the local atomic structure of defects with unpaired spins such as the silicon dangling-bond (db). However, the assignment of the EPR signal to a specific defect structure requires comparison to theoretical models.

Using density-functional theory, we address structure-property relationships by combining systematic studies for idealized db models in c-Si with a statistical analysis of a variety of dbs in a-Si:H supercells. Our studies reveal the influence of the local geometry on sp-hybridization and delocalization. Yet, the structural variability of a-Si:H cannot be captured by these idealized defect models alone. Rather, our calculations indicate that a relatively broad distribution of db-like structures gives rise to the experimental signal supporting a recent re-evaluation of EPR parameters from multi-frequency EPR [1]. Furthermore, to investigate how the stability of the dbs is affected by residual strain fields, we apply external strain to our crystalline and amorphous db models and monitor the evolution of structure and EPR properties.

[1] M. Fehr (et al.), Phys. Rev. B (in press), <http://arxiv.org/abs/1103.5641>

HL 40.2 Tue 11:45 EW 015

Vibrational spectra of charged point defects in ionic oxides — JIANCHUAN WANG, ●CHRISTOPH FREYSOLDT, and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung, Düsseldorf

We report calculations of the vibrational spectra of point defects which include the complete coupling to the host matrix. Such couplings are expected for charged defects in oxides and other ionic materials due to the long-range nature of electrostatic interactions. The dynamical matrix is computed from an electro-elastic model which combines long-range electrostatic forces with a pairwise interatomic harmonic correction for a limited number of neighbors. The model parameters are obtained from a few accurate density-functional theory *ground-state* calculations, requiring only forces and potentials which are readily available. Available symmetries are fully exploited. The approach is demonstrated for the +2 O vacancy in MgO. We show that the presence of the defect breaks the symmetry of the Born effective charge tensor of nearby atoms, and discuss the relevant sum rules. We also analyse how the defect modifies the vibrational density of states.

HL 40.3 Tue 12:00 EW 015

Evidence for Fe²⁺ in Wurtzite Coordination: Iron Doping Stabilizes ZnO Nanoparticles — ●JIANPING XIAO^{1,2}, AGNIESZKA KUC², SUMAN POKHREL³, MARCO SCHOWALTER⁴, SATYAM PARLAPALI⁴, ANDREAS ROSENAUER⁴, THOMAS FRAUENHEIM¹, LUTZ MÄDLER³, LARS PETTERSSON⁵, and THOMAS HEINE² — ¹Bremen Centre for Computational Materials Science, Bremen, Germany — ²School of Engineering and Science, Jacobs University Bremen, Germany — ³IWT Foundation Institute of Materials Science, Bremen, Germany — ⁴Institute for Solid State Physics, Bremen, Germany — ⁵Stockholm University, Stockholm, Sweden

First-principles calculations are used to investigate the structural and electronic properties of Fe-doped ZnO nanoparticles. Based on extensive validation studies surveying various density functionals, the hybrid functional PBE0 is employed to calculate the structures, formation energies, and electronic properties of Fe in ZnO with Fe concentrations of 6.25, 12.5, and 18.75 at%. Substitution of Zn by Fe, zinc vacancies, and interstitial oxygen defects is studied. High-resolution inner-shell electron energy loss spectroscopy measurements and X-ray absorption near-edge structure calculations of Fe and O atoms are performed. The results show that Fe-doped ZnO nanoparticles are structurally and energetically more stable than the isolated FeO (rocksalt) and ZnO (wurtzite) phases. The Fe dopants do not significantly alter the host ZnO lattice parameters. Simulations of the absorption spectra demonstrate that Fe²⁺ dominates in the Fe-doped ZnO nanoparticles

reported recently, whereas Fe³⁺ is present only as a trace.

HL 40.4 Tue 12:15 EW 015

Defects in amorphous silicon nitrides: Si₃N₄-Si₃N_x — ●LEIF ERIC HINTZSCHE, GEORG KRESSE, MARTIJN MARSMANN, GERALD JORDAN, CHANGMING FANG, and THOMAS WATTS — Computational Materials Physics, University of Vienna, Sensengasse 8/12, 1090 Vienna, Austria

Amorphous silicon nitride is widely used for memory and photovoltaic devices. In solar cells, it serves as a passivation and antireflection layer. In most cases, the silicon nitride layers are not stoichiometric and contain significant amounts of hydrogen. Currently, it is not well understood what distinguishes a good passivation layer that minimizes reflection losses from a bad passivation layer. To gain a more detailed atomic scale understanding, we present a careful study of the electronic properties of stoichiometric and non-stoichiometric silicon nitrides in the range of Si₃N₅-Si₃N₃. For each stoichiometry, several structural models are created containing typically 100 Si atoms. The evolution of the band gap, participation ratio, as well as the geometric and electronic defects states are analysed in detail. For the preparation of the structures, simulated annealing combined with standard density functional theory is applied, whereas the Heyd-Scuseria-Ernzerhof hybrid functional is used to analyse the electronic properties of the final structures.

HL 40.5 Tue 12:30 EW 015

Charge Carrier Density Control in In-based Multi Compound Solution Processed Oxide TFTs — ●MARLIS ORTEL, MARKO MARINKOVIC, GESA HELMS, and VEIT WAGNER — Jacobs University Bremen, School of Engineering and Science, Campus Ring 8, 28759 Bremen, Germany

Novel oxide semiconductors have recently caught much attention for TFTs in high-end 3D-TVs and smart-sensor applications. Materials like In-Ga-Zn-O (IGZO) show very high mobility, transparency and they are solution processable. When electrical stress is applied the TFT characteristics shifts. A reason for this instability are oxygen vacancies, which are attributed to weak indium-oxygen bonds. The vacancies result in traps and doping of the active layer.

In this work charge carrier control in TFTs by addition of Al and Si to indium oxide was investigated. These components were chosen with respect to the bonding properties to oxygen. Si and Al show almost the same ionic radius but differ in the bond dissociation energy to oxygen by a factor of 1.6. A systematic influence on the charge carrier density caused by oxygen vacancies is expected. For the investigation TFTs were electrically and morphologically characterized. The analysis gave a high mobility of 12cm²/Vs for the In-Al-O material system. The density of deep trap states near the mid-gap was analyzed to be 6.8E12eV⁻¹cm⁻² in In-Al-O and as low as 2.2E12 eV⁻¹cm⁻² in the In-Si-O material system.

In conclusion addition of silicon is a proper method to control the bulk charge carrier density, i. e. doping level, in In-based oxide TFTs.

HL 40.6 Tue 12:45 EW 015

THz spectroscopy of the 29 cm⁻¹ oxygen vibrational line in natural silicon and isotopically enriched ²⁸Si — ●KURT LASSMANN¹, BORIS GORSHUNOV^{1,2,3}, P.S. KOROLEV^{2,4}, E.S. ZHUKOVA^{1,2,3}, V.P. KALINSUKHIN², N.V. ABROSIMOV⁵, P.G. SENNIKOV⁶, H.-J. POHL⁷, S. ZAKEL⁸, and MARTIN DRESSEL¹ — ¹Phys. Inst., Univ. Stuttgart — ²A.M. Prokhorov Gen. Phys. Inst., RAS, Moscow — ³Moscow Inst. Physics and Technology — ⁴Lomonosov Moscow State Univ. — ⁵Leibniz Inst. Kristallzüchtung, Berlin — ⁶Inst. Chem. High-Purity Substances, Nizhny Novgorod — ⁷PTB, Braunschweig — ⁸VITCON-Projektconsult, Jena

Looking for a possible host-isotope effect on the low-energy two-dimensional motion of interstitial oxygen in silicon we have measured the resonance parameters of the lowest transition of the 30 cm⁻¹ band of the Si-O-Si complex in natural Si and in isotopically enriched ²⁸Si at temperatures between 5 K and 22 K by means of coherent-source terahertz spectroscopy. At 5.5 K we obtain for the resonance maxima 29.24 ± 0.003 cm⁻¹ and 29.22 ± 0.003 cm⁻¹ and for the line widths 0.09 ± 0.01 cm⁻¹ and 0.11 ± 0.01 cm⁻¹ for ²⁸Si and natSi, respectively. Both lines can be fitted by single Lorentzians, so, no obvious isotopic

structure or asymmetry of the line in ^{nat}Si due to the Si neighbors in the Si-O-Si complex is detected. We therefore conclude that down-shift and broadening of the ^{nat}Si -resonance is not due to the Si isotopes in the isolated Si-O-Si complex but to an average effect of the isotopically inhomogeneous lattice.

HL 40.7 Tue 13:00 EW 015

Diffusion of Cu (I) in amorphous In_2S_3 thin films investigated by Rutherford backscattering spectroscopy — ●ALBERT JUMA¹, PAUL PISTOR¹, THOMAS DITTRICH¹, and ELKE WENDLER² — ¹Helmholtz-Centre Berlin for Material and Energy, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — ²Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Amorphous In_2S_3 thin films can be used in charge-selective layer sys-

tems for example in contact with chalcopyrite absorber or in contact with CuSCN hole conductor. Diffusion of Cu (I) plays a crucial role for the electronic properties of charge-selective contact systems with In_2S_3 . In our experiments CuSCN was sprayed as a Cu (I) source on evaporated amorphous In_2S_3 thin films (layer thickness 100 nm) and the annealing temperature was varied and annealing time was fixed. After annealing CuSCN was etched away in pyridine solution. The Cu concentration profiles were obtained from Rutherford backscattering (He^+) measurements. Temperature dependent diffusion coefficients were deduced from the measurements. The value of the exponential prefactor was of the order of $10^8 \text{ cm}^2\text{s}^{-1}$ and the activation energy amounted to about 0.9 eV. A suggestion on the diffusion mechanism will be drawn.