8:30-8:45
Oral: Hermann Detz
Atomistic Modeling of Bond Lengths in Ternary III-V Semiconductor Alloy

We present atomistic simulations of III-V semiconductor materials based on empirical interaction potentials. The ternary alloys InGaAs, InAlAs and GaAsSb were used as model systems. Chemical bonds were modeled with the Tersoff potential, where parameter sets for binary compounds were evaluated with respect to their suitability in ternary alloys. Atoms were placed in ideal zincblende lattice cubes with an edge length of six unit cells and relaxed using a Metropolis Monte Carlo solver. The bulk and shear moduli served as figures of merit and could be reproduced with a maximum error of 5 % and 13 %, over the whole composition range. A modified solver scheme allows to model thermal expansion, by reducing the error to 25 %, compared to previous works.

In addition to random alloys, we also investigated CuPt-ordered ternary alloys, where the constituent binaries are stacked along the [111] axis. Such ordered structures were observed experimentally and are known to influence material properties and device characteristics. While random alloys led to broad bimodal bondlength distributions, CuPt-ordered structures showed four distinct peaks. These correspond to one perpendicular and three in-plane bonds, which is reflected in the peak area ratio of 1:3:3:1. One binary is compressed within the (111) planes and stretched perpendicular to these and vice versa, leading to a deformed lattice with inherent strain up to 1.8 %. Softer materials show broader peaks, for a random alloy but sharper peaks for CuPt-ordered structures.

Co-authors: Gottfried Strasser

8:45-9:00
Oral: Naoki Matsushima
First Principles Study on X-Ray Photoelectron Spectroscopy Binding Energies of Nitrogen in Silicon Carbide

We studied the X-ray photoelectron spectroscopy (XPS) binding energy of nitrogen (N) defects in silicon carbide (SiC) using the first principles calculation.
Recently, the high intensity X-ray beams generated by large synchrotron radiation facilities have enabled detailed XPS measurements of lattice defects. While the XPS can give the information of the atomic-scale structure, theoretical calculations are required to analyze the XPS spectra.
The SiC is a candidate for the substrate of efficient power devices. The N is an n-type dopant in SiC. However, it is known that the N-doped SiC shows a saturation of the electrical activation in high concentration. This saturation is considered due to the formation of the