Electronic Raman Scattering of Phosphorus Donors in Silicon Carbide — Martin Hundhausen, Roland Puesche, and Lothar Ley — Technische Physik, Universität Erlangen

We have studied temperature and polarization dependent electronic Raman scattering in phosphorus doped Silicon Carbide (SiC). We observe signals in the low temperature Raman spectra with Raman shifts between 2.2 meV and 5.3 meV depending on the polytype. We assign these energies to transitions between the donor 1s ground state to its valley-orbit split 1s excited state. Different valley-orbit energies are assigned to signals originating from donors substituting different inequivalent lattice sites of host Si atoms. The splitting results from the different symmetries of possible linear combinations of states at the nonequivalent conduction band minima of SiC. From the polarization dependence of the Raman signals for 6H- and 4H-SiC we conclude that the two possible 1s donor states belong to $E_2$ and $A_1$-symmetry of the $C_6v$ point group of the crystal, respectively. The temperature dependent occupation of these states as monitored by the Stokes and Anti-Stokes intensities in the Raman spectra in combination with the known degeneracies $g_{A1}$ and $g_{E2}$ suggests that the $A_1$ state is the ground state.

Electronic properties of the 2x1 3C-SiC surface reconstruction studied with resonant photoemission — Massimo Tallarida, Rakesh Sohal, and Dieter Schmeisser — Angewandte Physik-Sensorik, Brandenburgische Technische Universität, Konrad Wachsmann Allee, 17-03046-Cottbus

We have studied the 2x1 reconstructed surface of the 3C-SiC polytype by means of photoemission spectroscopy. The reconstruction was characterized through Si2p and C1s core level and angle-integrated valence band spectroscopy, and confirmed by the observation of a two-domain 2x1 LEED pattern. The electronic properties of this surface were investigated by collecting valence band spectra at photon energies near the Si2p and C1s absorption edges. The results show a strong dependence of the photoemission intensity on the excitation energy with characteristic resonances for certain valence band features. With a detailed study of the resonances we are able to assign the electronic origin of the resonating states and the nature of the electronic transition near the absorption edges.

Kinetic mechanisms for the deactivation of nitrogen — Alexander Mattausch, Michel Bockstedte, and Oleg Pankratov — Theoretische Festkörperphysik, Staudtstr. 7/B2, 91058 Erlangen, Germany

Nitrogen is a common dopant in silicon carbide. It is known that nitrogen substitutes for carbon atoms. Yet surprisingly, recent experiments have shown [1] that the silicon co-implantation (which should support N incorporation on the C-sublattice) leads to a significant deactivation of nitrogen at high annealing temperatures. At the same time, the concentration of compensating centers decreases. Employing ab initio density functional theory calculations we investigate the interaction of the nitrogen dopants with self-interstitials and vacancy aggregates in 4H-SiC. We find that a silicon interstitial can kick-out the activated N$_C$, since the emission of a nitrogen interstitial from the (N-Si)$_C$ complex is favoured over the silicon emission by 1 eV. The reaction of N with carbon interstitials leads to (CN)-complexes which possess deep levels. These defects have dissociation energies between 2.6 eV and 3.2 eV and thus are thermally stable. Yet, the formation of these complexes requires moderate temperatures and cannot be responsible for the high temperature annealing behaviour after silicon co-implantation. A possible alternative is the formation of the highly stable vacancy clusters (V$_C$)$_n$-V$_Si$. Due to the high migration barrier of V$_C$ this process is possible only at high temperatures. These defects can trap nitrogen interstitials, finally leading to the electrically passive (N$_C$)$_4$V$_Si$ complexes.