Abstract
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„Radiation-induced Defects in Silicon Carbide: Investigations with Optically Detected Electron-Paramagnetic Resonance“

Radiation-induced point defects in silicon carbide (SiC) were investigated using electron-paramagnetic resonance (EPR), photoluminescence (PL), the magnetic circular dichroism of the absorption (MCDA) and optically detected magnetic resonance (MCDA-EPR and PL-EPR).

In neutron-irradiated samples annealed beyond the annealing temperature of the isolated silicon vacancy, EPR spectra of spin $S = 1$ centers were observed that have the symmetry of nearest neighbor pair defects. EPR spectra of the defect on the three inequivalent lattice sites were resolved and attributed to optical transitions between photon energies of 999 meV and 1075 meV by MCDA-EPR. The hyperfine structure of the EPR spectra shows the presence of one single carbon nucleus and several silicon ligand nuclei. The experimental findings are interpreted with help of total energy and spin density data obtained from the standard local-density approximation of the density-functional theory (LSDA-DFT), using relaxed defect geometries obtained from the selfconsistent charge density-functional theory based tight binding (SCC-DFTB) scheme. The calculations were performed by the department of theoretical physics at the University of Paderborn (E. Rauls, U. Gerstmann, and H. Overhof). The only model that explains all experimental findings is the photo-excited spin triplet state of the carbon antisite - carbon vacancy pair (C_{Si}-V_C) in the doubly positive charge state. It is concluded that the C_{Si}-V_C defect is formed from the isolated silicon vacancy as an annealing product by the movement of a carbon neighbor into the vacancy.

The optical transitions of a radiation-induced defect that is presently assigned to the silicon vacancy in the neutral charge state were investigated in 6H- and 15R-SiC with the MCDA method. Only the quasicubic sites of the defect give rise to a MCDA signal whereas the hexagonal sites do not. The temperature and magnetic field dependence of the MCDA lines indicates a spin $S = 1/2$ for the ground state of the quasicubic sites, in contrast to published models. The MCDA-EPR signals of the quasicubic sites also differ from the published signals measured with PL-EPR. It is suggested that the charge transfer levels of the silicon vacancy at the quasicubic sites differs from the hexagonal sites, so that the quasicubic sites exist in other charge and spin states than the hexagonal sites.

The so-called D1 center is a common radiation-induced defect in all polytypes of SiC. Its PL spectrum is frequently observed after irradiation and subsequent annealing and has been known for 30 years, but the microscopic structure of the defect is to date unidentified. This center was investigated with PL-EPR. Its magneto-optical properties indicate a paramagnetic behavior of the defect, in agreement with published data from Zeeman experiments. But despite the use of modern spectroscopic methods like high frequency EPR and EPR detected via the magnetic circular polarization of the emission (MCPE), no EPR signal could be

assigned to the defect. Based on the present understanding of the defect, the silicon antisite is suggested as a suitable model for the D1 center.