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Defect related electrical and optical properties of AlN bulk crystals grown by physical vapor transport

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AlN crystallizes thermodynamically stable in the wurtzite structure and possesses a direct band gap of about 6 eV. It is the ideal substrate for the epitaxial growth of Al-rich $Al_xGa_{1-x}N$ films that enable deep ultraviolet (UV) emitters. Appropriate AlN bulk crystals can be grown by physical vapor transport (PVT). Besides high structural perfection, such substrate crystals should be highly UV transparent and ideally, electrically conductive. It is well known that point defects like impurities and intrinsic defects may introduce electronic energy levels within the bandgap, which lead to additional optical absorption or electrical compensation. Among the impurities, which may be incorporated into the AlN crystals during PVT growth at well above 2000 C, oxygen, carbon, and silicon play the major role. Based on our own experimental data as well as on experimental and theoretical results reported in literature, we discuss energy levels, charge states and possible negative-U behavior of these impurities and of vacancy-type defects. In particular, we develop a model that explains the absorption behavior of the crystals in dependence on the Fermi level that can be controlled by the growth conditions, including intentional doping. Further, we pay attention on spectroscopic investigations giving direct evidence for the chemical nature and atomic arrangement of the involved point defects. As examples local vibrational mode (LVM) spectroscopy of carbon related defects and recent reports of electron paramagnetic resonance (EPR) spectroscopy are discussed.