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THE CORE STRUCTURE OF A 30 DEGREE PARTIAL DISLOCATION IN GaAs: MERGING THEORY AND EXPERIMENT QUANTITATIVELY

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In recent years it became possible to extent the resolution of field emission microscopes into the sub Angstrom region by reconstruction of the electron exit wave from a focal series of lattice images. Thereby, it is now feasible to investigate defects and interfaces on a truly atomic scale in many materials systems. On the other hand, progress in theory enables scientists to calculate the total energy configuration of systems that are comparable in size with what is typically investigated by high-resolution transmission electron microscopy. Therefore, a quantitative investigation of the agreement between theoretical calculations and experiments is feasible. In this contribution we investigate the core structure of a 30-degree partial dislocation in low temperature grown GaAs:Be. Ab initio electronic structure total energy calculations are used to compute the expected structure for both the Ga-centered and the As-centered 30 degree partial dislocation cores in GaAs. NCEM's One Angstrom Microscope with an information limit of ~ 0.08 nm is used to image this structure. It is shown that it is possible to discriminate between Ga and As columns in phase contrast microscopy if wedge shaped samples are utilized. The agreement between theory and experiment is tested by a determination of the column position in - and around the dislocation core with pico meter precision. The agreement between experiment and theory is remarkable. Currently, strain relaxation and column bending in the ~ 5nm thin TEM foil are major sources of difference between calculations and experiments and they are accessed quantitatively.

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