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Modeling of Threading Dislocation Core Fields and of Point Defects in GaN JENNIFER R. SNIVELY, Wright State University, Dayton OH, STEFAN C. BADESCU, Air Force Research Laboratory, WPAFB OH — Point defects and dislocations in GaN are involved in failure mechanisms of GaN-based electronic devices. Compared to bulk material, the electronic states and diffusivities of point defects are modified by dislocation elastic fields. For accurate descriptions atomistic calculations have to take into account both the long (Volterra) and the short-range components of the latter. We present an atomistic picture of defect energy levels and diffusion barriers for vacancies, interstitials and impurities next to threading dislocations in GaN. We include the dislocation core field derived from stress calculations using periodic supercells. We show that this increases significantly the point defect-dislocation interaction by comparison to the Volterra field and that the diffusion energy barriers are changed by as much as 50%. The dependence of charged energy levels on the Fermi level is also modified on many lattice spacings away from the dislocations. We discuss in more detail the charged N vacancies and the Ga and Al interstitials.

Stefan C. Badescu
Air Force Research Laboratory, WPAFB OH

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