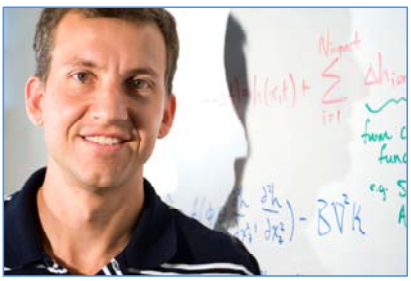
Understanding Electrical and Optical Effects of Dislocations in III-V Semiconductors

The electrical and optical properties of group III-V semiconductor alloys have vastly different sensitivities to the presence of dislocations. Some materials, like GaAs, have severely degraded photoluminescence intensity in the presence of even low dislocation densities, while other materials, like GaN, have a robust optical response when the dislocation density is many orders of magnitude larger. In this talk, a theoretical framework is presented for studying the effects of dislocations in these materials. Dislocations are first studied using ab initio atomistic methods in order to determine the electronic structure of the core. Then each dislocation is treated using classical electrostatics, whereby a screened potential is assigned to mimic the effect of the dangling bonds along the dislocation line. The optical properties are then studied using a multi-band effective mass model to compute the electron energy levels, the density of states, and ultimately the optical emission spectra of a sample of material containing an array of dislocations. Electron mobility is computed separately by means of a classical scattering model incorporating the dislocation electrostatic potential. A wide range of experimental results are then predicted and interpreted based on the computational model, especially for the interesting case of GaN. Finally, the wide disparity in the dislocation sensitivity between GaN and GaAs is explained in the context of this new model.



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Harley Johnson is an Associate Professor in the Department of Mechanical Science and Engineering. His research is in the area of mechanics of electronic materials, nanostructures, and materials for nanophotonics, with a specific focus on understanding coupling between mechanical, electronic, and optical properties of these systems. He is active in the Materials Research Society, the American Society of Mechanical Engineers, and the American Physical Society; he is also the General Chair of the 2008 Annual Conference of the Society of Engineering Science, to be held at the University of Illinois. He received the NSF CAREER Award in 2001, and has been a Cannon Faculty Scholar in Mechanical Engineering since 2003.