ID: 12.1b

Title: First-Principles Studies of Loss Mechanisms in Nitride Light Emitters

Name: Van de Walle, Chris

Affiliation: Materials Department, University of California, Santa Barbara

Indium gallium nitride alloys are successfully being used for light emitting diodes (LEDs) and laser diodes (LDs) in the green to ultraviolet part of the optical spectrum. These devices are the key enablers to Solid-State Lighting, which promises to significantly cut electricity consumption. Applications are still limited, however, by the declining efficiency of LEDs at high currents (?droop?) and by absorption losses of undetermined origin in LDs. Several mechanisms have been suggested as the cause of this efficiency loss, such as Auger recombination and free carrier absorption. Experimentally it is very difficult to discriminate between different nonradiative processes. We have therefore addressed the loss mechanisms based on state-of-the-art first-principles computational theory. We use ab initio wave functions and bands that are accurate throughout the entire Brillouin zone (as opposed to k.p band structures). For free-carrier absorption, we discovered that the relevant optical processes are indirect. The indirect absorption of light, despite being an important optical process in many materials, had not been investigated with fully first-principles calculations before. Various scattering mechanisms have been taken into account, including scattering by alloying, defects, and phonons. The electron-phonon coupling is explicitly evaluated; this interaction is usually modelled by the Frˆhlich expression and this is the first time that the validity of this model is verified from ab initio data. We determine the optical absorption coefficient and the corresponding photon mean free path as a function of carrier concentration. The computed values indicate that the effect is weak in LEDs but constitutes an important loss mechanism in LDs. For Auger recombination we find that both electron-electron-hole and hole-hole-electron processes contribute, and that indirect processes assisted by alloy scattering and by electron-phonon coupling dominate. The magnitude of the resulting Auger coefficient indicates that Auger recombination is indeed responsible for the efficiency reduction at high carrier densities. Strategies for overcoming this limitation will be discussed. Work performed in collaboration with E. Kioupakis, P. Rinke, and K. Delaney.