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Quasi-localized states, electron scattering and carrier mobility in GaNAs[1]

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Mobility of n-type carriers is an important determining characteristic of the dilute nitride semiconductors. The introduction of small amounts of nitrogen, which is so effective in reducing the band-gap, also drastically reduces the mobility of GaAs. Solar power applications are limited by the low carrier mobility (typically $\sim 200\ \mathrm{cm}^2(Vs)^{-1}$) and an understanding of the microscopic mechanisms governing transport could lead to substantial improvements in growth methods. The strong perturbation to the low-lying conduction bands by substitutional nitrogen makes a theoretical treatment of carrier transport difficult in these systems. Using a combination of parameterized tight-binding calculations of GaNAs, which allow us to accurately describe the energies and wavefunctions of electronic states in the low-lying conduction bands, we characterize the electronic states near the conduction band edge as a linear combination of isolated nitrogen states and GaAs conduction band states. Using the resulting spectrum of quasi-localized states coupled to itinerant states of the GaAs host, we calculate the effect of alloy scattering on the n-type carrier mobility in the regime of degenerate and non-degenerate doping within a resonant scattering approach and the relaxation time approximation to the Boltzmann transport equation. Excellent agreement is found with measured values of the mobility. By analysing scattering from different states in the spectrum of quasi-localized states, we identify scattering by random clusters of nitrogen atoms (i.e. nitrogen atoms which share Ga nearest -neighbours) as a major limiting factor on the mobility.

[1] work pertormed in collaboration with A. Lindsay, H. Ouerdane, and E. P. O'Reilly,