Monte Carlo Study of Transport Properties of InN

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In recent years Indium Nitride has attracted much attention due to the considerable advancement in the growth of high quality crystals. Furthermore, several new works on the material properties proposed a bandgap of 0.7 eV [1,2], instead of about 2.0 eV as believed before. Thus, previous electron transport models have to be re-examined, in respect of the new band structure. We use a Monte Carlo approach to investigate the electron transport in InN. Our single-particle technique includes the three lowest valleys of the conduction band (G1, G3 and M-L) and accounts for non-parabolicity of the main valley. Several stochastic mechanisms such as acoustic phonon, polar optical phonon, inter-valley phonon, and ionized impurity scattering are considered and their impact is assessed. An accurate piezoelectric scattering model, which accounts for non-parabolicity and wurtzite material structure is also employed [3]. This is especially important since nitrides exhibit the largest piezoelectric constants among the III-V semiconductors. Considering the wurtzite structure we adopt the corresponding elastic constants and piezo coefficients [4]. Simulations with two different setups are conducted: one with a bandgap of 1.89 eV (effective mass $0.11m_0$ in the G1 valley [5]), and one with bandgap of 0.69 eV (effective mass of $0.04m_0$ [6]). Results for electron mobility as a function of lattice temperature, free carrier concentration, and electric field were obtained. For example, Figure 1 shows the low-field electron mobility in hexagonal InN as a function of free carrier concentration. Results from other groups and various experiments are also included. Assessing the classical band structure model (Eg=1.89 eV), we achieve electron mobility reaching 4500 cm^2/Vs, which is in a good agreement with the theoretical results of other groups using the same setup (Chin, et al. [7]). Considering the newly calculated band structure model (Eg=0.69 eV), maximum mobility of about 10000 cm^2/Vs is achieved. This increase has to be explained with the lower effective electron mass. Polyakov, et al. [8] calculated a theoretical limit as high as 14000 cm^2/Vs, however their simulation does not account for piezoelectric scattering, which has an important role at lower concentrations.

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