Majority and Minority Mobilities in Heavily Doped Gallium Aluminum Arsenide for Device Simulations

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ABSTRACT

Simulators for heterojunction bipolar transistors (HBTs) require physical models and associated input parameters that describe how carrier transport varies with carrier concentrations, ionized dopant densities, alloy mole fractions, and temperature. In order to increase the probability that simulations of HBTs are predictive and useful for the future development of HBTs, accurate and independent values for the majority and minority mobilities of electrons and holes in $Ga_{1-y}Al_yAs$ are essential for reducing the number of unknown or fitting parameters. The majority electron and minority hole mobilities in $Ga_{1-y}Al_yAs$ for donor densities, N_d, between 10^{16} cm^{-3} and 10^{19} cm^{-3} are calculated by first-principles methods based on quantum mechanics.[1] Similarly, the majority hole and minority electron mobilities for acceptor densities, N_a, between 10^{16} cm^{-3} and 10^{20} cm^{-3} are calculated. The mole fraction of AlAs, y, varies between 0.0 and 0.3 in these calculations. All the important scattering mechanisms for low-field mobilities are included; namely, alloy scattering, acoustic phonon, polar optic phonon, nonpolar optic phonon (holes only), piezoelectric, ionized impurity, carrier-carrier, and plasmon scattering. The ionized impurity and carrier-carrier scattering processes are treated with a quantum-mechanical, phase-shift analysis. These calculations are the first to use a phase-shift analysis for minority carriers scattering from majority carriers in ternary compounds such as $Ga_{1-y}Al_yAs$.

The Boltzmann transport equation is solved by the variational procedure outlined by Walukiewicz *et al.*[2] This method avoids the use of the relaxation-time approximation that is invalid for mechanisms that involve energy transfers comparable to or greater than k_BT, where k_B is Boltzmann's constant and T is absolute temperature. Matthiesson's rule also is not used since it is not valid for $Ga_{1-y}Al_yAs$. The scattering rates are summed prior to the variational solution. The results are highly accurate calculations of the mobilities for $Ga_{1-y}Al_yAs$ as functions of the dopant density and the mole fraction of AlAs. The calculated results agree well with the rather limited experimental data for $Ga_{1-y}Al_yAs$ majority mobilities and predict that at high dopant densities minority mobilities should increase with increasing dopant density for a short range of densities. This effect occurs because of the reduction of plasmon scattering and the removal of carriers from carrier-carrier scattering due to the Pauli exclusion principle. The above approach for calculating scattering mechanisms also has implications for the scattering cross sections used in Monte-Carlo calculations to treat heterostructure devices. The application of these methods to Monte-Carlo calculations should yield more accurate values for the velocity-field relations.

The input parameters for these calculations are the alloy scattering potential, bandgap, carrier masses, dielectric constants, lattice constant, mass density, phonon energies, elastic tensor elements, and piezoelectric coefficients. The variations of these parameters with y are given by Adachi.[3] The alloy scattering is treated as the scattering of carriers by a square well potential with a depth approximated by the corresponding band edge shift and with a width somewhat arbitrarily taken to be the nearest-neighbor separation.[4] Figures 1 to 4 show the results for the

majority and minority electron mobilities. None of the input parameters were varied to fit the experimental data given in Figure 2. The mobility ratios given in Figure 4 are quantitatively significant for simulations of HBTs. Most simulations of HBTs use majority mobility values for corresponding minority mobilities. Qualitatively similar results are obtained for the hole mobilities.

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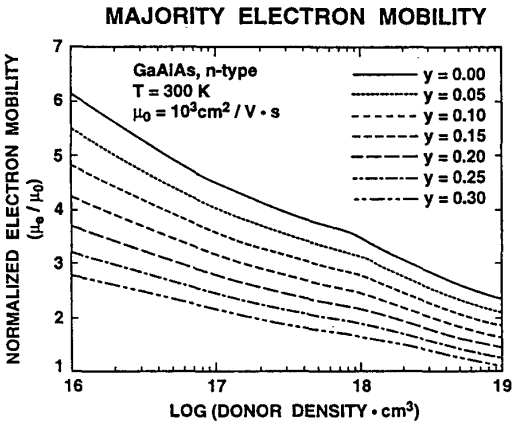

Figure 1

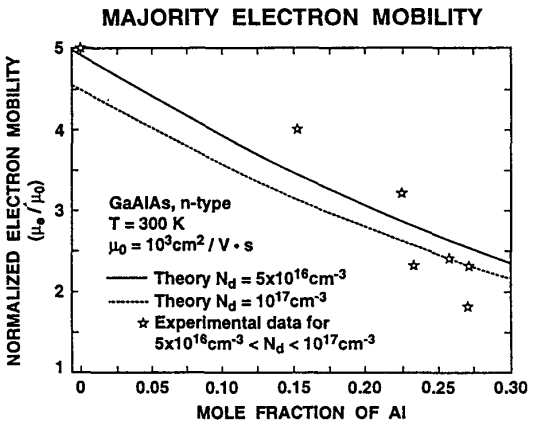

Figure 2

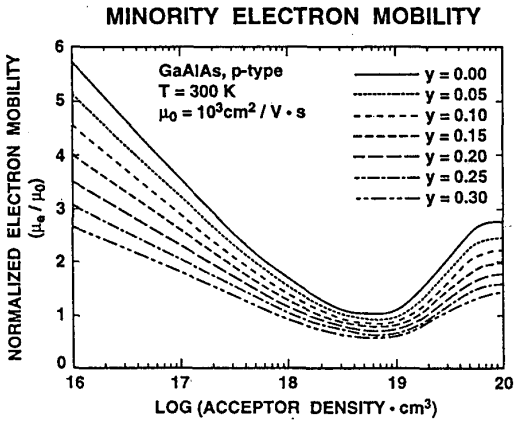

Figure 3

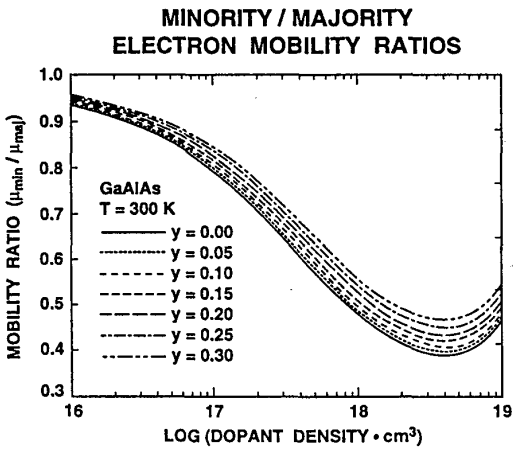

Figure 4