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Solution of Boltzmann equation for calculating the Hall mobility in bulk GaN_xAs_{1-x}

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Introduction

Although considerable attention has been given to theoretical models of the band-structure in dilute nitrides[i-iv] until recently there has been very little development in the theory of carrier transport[v],[vi]. Studies that have been carried out based on a relaxation time approximation[v] suggest that there may be intrinsic limits on electron mobility, which will be an important consideration for device applications.

The effect of the high degree of non-parabolicity in the energy dispersion relations predicted by the band-anticrossing (BAC) model has not yet been addressed. Nor have other scattering mechanisms been considered, particularly polar optical scattering, which can not be treated using a relaxation time approximation due to the highly inelastic nature of the interaction.

We have developed the ladder method[vii],[viii] for solving the Boltzmann equation to deal with a non-parabolic, spherical conduction band. Using the BAC model to calculate the modified effective mass and density of states, we have calculated the low field Hall mobilities for bulk GaN_xAs_{1-x}.

The rate for scattering from nitrogen centres has been derived from the scattering matrix due to Fahy and O'Reilly[v].

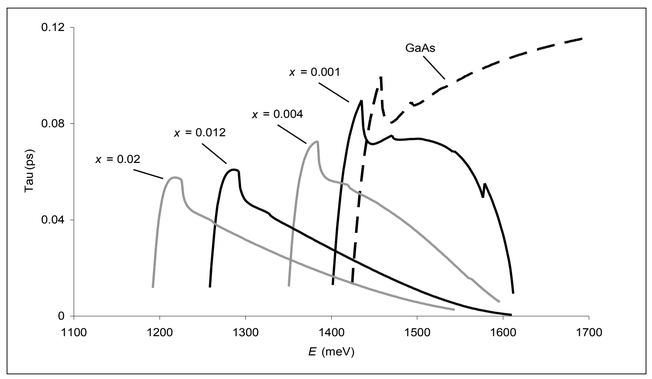

Figure 1 Relaxation times for all scattering processes at different nitrogen concentrations. The discontinuities are due to the ladder nature of polar optical scattering. Note that the relaxation times all tend to zero near the nitrogen level. Also shown for comparison is the relaxation time for GaAs with the same donor and acceptor doping ($N_D = 10^{17}$ cm^3, $N_A/N_D = 0.5$).

Results

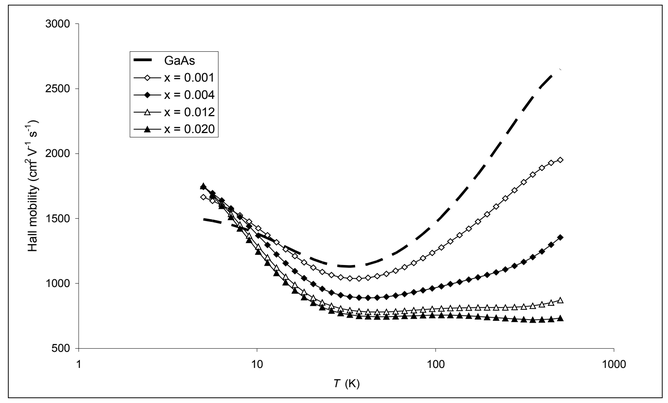

Figure 2 Hall mobility for GaN_xAs_{1-x} for different nitrogen concentrations. In each case, the donor concentration is $N_D = 10^{17}$ cm^{-3} and the compensation ratio is $N_A/N_D = 0.5$. The mobility for GaAs is shown for comparison (dashed line).

Figure 1 shows the calculated relaxation times at 300 K. The discontinuities at energy separations of the phonon energy are a characteristic feature of the ladder method. In general, the scattering rates at an energy E are correlated to the rates at energies $E€± €ħω$. However, for $E€<€ħω$ there is no possibility of phonon emission, so the rate changes discontinuously at $E = ħω$ with the effect being propagated further up the ladder. The most obvious effect of the non-parabolicity is the tendency of the relaxation times towards zero near the nitrogen energy, where the electron becomes immobile.

In figure 2 we show the temperature dependence of the calculated Hall mobility (in a 0.5 T magnetic field) for various nitrogen concentrations. At this level of doping, neutral and ionised impurity scattering tend to be dominant at low temperatures, with the mobility only curving over at high temperature (characteristic of polar optical limited transport) for low values of x. For $x€>$ 0.004, the high temperature mobility becomes limited by nitrogen scattering.

The contributions of the individual processes are illustrated in figure 3 for x = 0.02. At this nitrogen concentration, nitrogen scattering pins the high temperature mobility to around 720 cm^{-2} V^{-1} s^{-1}.

Conclusions

Despite the large reduction in mobility compared to GaAs, these results are still about an order of magnitude larger than many of the experimental determinations of the Hall mobility in compensated GaInNAs[ix],[x], although electron mobilities of up to 2000 cm^{2}V^{-1}s^{-1} have been reported[xi]. Moreover, the results found here are of the same order of magnitude as the studies based on the relaxation time approximation for nitrogen scattering. This implies that the non-parabolicity of the conduction band predicted by the BAC model can not of its own explain the very low mobilities observed in dilute nitrides.

The model for nitrogen scattering used here is based on isolated nitrogen impurities. However, it has been pointed out by Fahy and O'Reilly[xii] that the effect of disorder due to different N environments needs to be considered and their calculations predict a resonant level close to the conduction band edge that may dominate the scattering.

It is clear that the introduction of N into III-V semiconductors has a serious effect on the mobility. These calculations suggest that for x > 0.001, upper limits of 1000 – 2000 cm^{2}V^{-1}s^{-1} may be imposed.

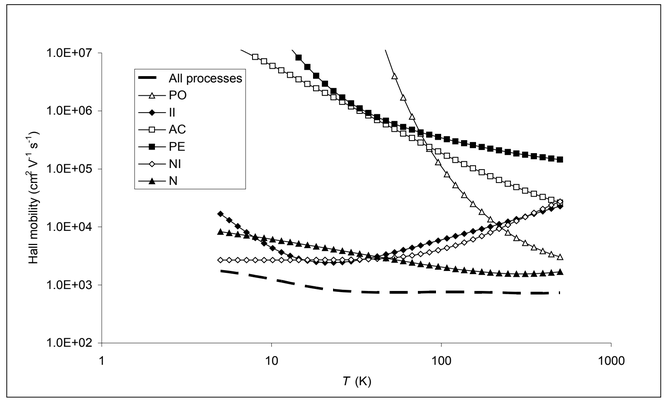

Figure 3 The components of the mobility due to separate processes for a nitrogen concentration of x = 0.02. Note that at low temperature, neutral impurity scattering dominates, whilst above about 40 K scattering from nitrogen centres is the dominant mechanism limiting the mobility.

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