Nitrogen-Induced Decrease of the Electron Effective Mass in $GaAs_{1-x}N_x$ Thin Films Measured by Thermomagnetic Transport Phenomena

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$GaAs_{1-x}N_x$ alloys have sparked a flurry of experimental[1] and theoretical[2] work based on their dramatic material property changes with dilute N concentrations. The decrease in optical bandgap down to ~1eV with < 3% N makes it a candidate for a middle cell in a multijunction solar cell.[3] Unfortunately, this drop in bandgap with increasing N concentration is also accompanied by a decreasing mobility. Previous experiments[4,5] have identified an increasing electron effective mass as the culprit for the poor mobilities, but lack of agreement between experimental techniques has left the question open for debate.

Effective mass measurements on low-mobility materials are notoriously difficult. This is due, in part, to short relaxation times. Cyclotron resonance techniques require the product $\omega\tau >> 1$ to be satisfied (a condition, admittedly, not met by the authors in ref. [6]), while optical resonance techniques are model[6] and input-parameter dependent.[4] Density-of-states effective mass (DOS m*) measurements on low-mobility samples ($\mu <$ 1200 $cm^2/V\text{-}s$) are best made with four transport coefficients[7,8] (resistivity, Hall, Seebeck, and Nernst), because the weak-field regime condition ($\mu B << 1$) is easily satisfied.[9]

In this paper, we present temperature-dependent resistivity, and Hall, Seebeck, and Nernst coefficient transport data[10] for 2-μm-thick thin films of $GaAs_{1-x}N_x$ grown on insulating GaAs substates by MOCVD. The films were Se doped to a carrier concentration of 5-7.6 $\times 10^{18}$ cm^{-3} while varying the N concentration from 0 — 0.4 % (x = 0.004). Samples with higher N concentrations were grown and characterized, but they required In incorporation to avoid cracking problems, and thus will not be included in this paper. Typical data are shown in Fig. 1. The room-temperature Hall mobility decreased from 1263 $cm^2/V\text{-}s$ for N = 0% to 187 $cm^2/V\text{-}s$ for N = 0.4%. This trend was accompanied by an increase in the Seebeck coefficient and a decrease in magnitude and change of sign in the Nernst coefficient. A change in sign of the Nernst coefficient can imply a change in the scattering mechanism, but further mapping of the nonparabolicity of the $GaAs_{1-x}N_x$ alloy conduction band (m*(n)) is needed to elucidate the scattering mechanism(s). Temperature-dependent Hall mobility data clearly show a change in scattering mechanism from ionized impurity-like to neutral impurity-like scattering with increasing N concentration.

DOS m* values were calculated using the equation[8]

$$m_d^* = \left(\frac{3}{|R_H|q\pi}\right)^{2/3} \frac{q\hbar^2}{k_B^2 T}\left(\alpha - \frac{Q}{|R_H|\sigma}\right),$$

where R_H is the Hall coefficient, σ the conductivity, α the Seebeck coefficient, Q the Nernst coefficient, T the absolute temperature, and k_B Boltzmann's constant. Fig. 2 shows the calculated DOS m* values for five $GaAs_{1-x}N_x$ samples with nitrogen concentrations from 0% — 0.4%. The pure GaAs sample has a DOS m* consistent with literature values for carrier concentrations of 5×10^{18} cm^{-3}.[11]

The most interesting feature of Fig. 2. is the *decreasing* DOS m* with increasing N concentration. This is the first report of effective mass values for dilute ($N \leq 0.4\%$) $GaAs_{1-x}N_x$, but it differs significantly from the previous reports[4,5] using $GaAs_{1-x}N_x$ /GaAs quantum well samples with higher N concentrations. Our data follow the same trend as ref. [5], but with lower values of DOS m* with respect to GaAs.

Our results may be explained by recognizing that two competing effects may be at work in GaAs. The first is the reduction of effective mass with decreasing bandgap caused by ordering within the alloy. The second is a mixing of conduction band states (Γ_{1c}, L_{1c},and X_{1c}), which alters the character of the lowest energy state.[12] As x increases, the L_{1c} state mixes with the Γ_{1c} state and strongly influences the character of the lowest energy conduction band. The L_{1c} state has a much larger m* than the Γ_{1c} state; hence, the DOS m* value increases.[13] Evidently, the first of these effects is predominant in dilute $GaAs_{1-x}N_x$, whereas the latter is stronger with higher N concentrations.

We conclude that low mobilities in dilute $GaAs_{1-x}N_x$ are due to short relaxation times rather than large DOS m* values.

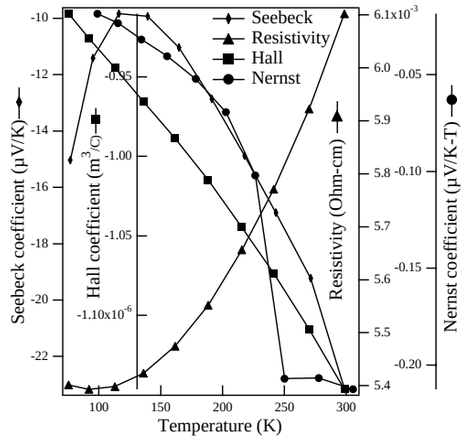

Figure 1. Transport data for $GaAs_{1-x}N_x$ (0.4% N)

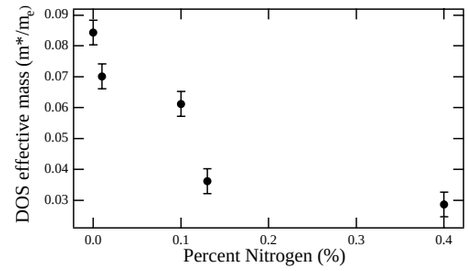

Figure 2. DOS m* vs N concentration

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