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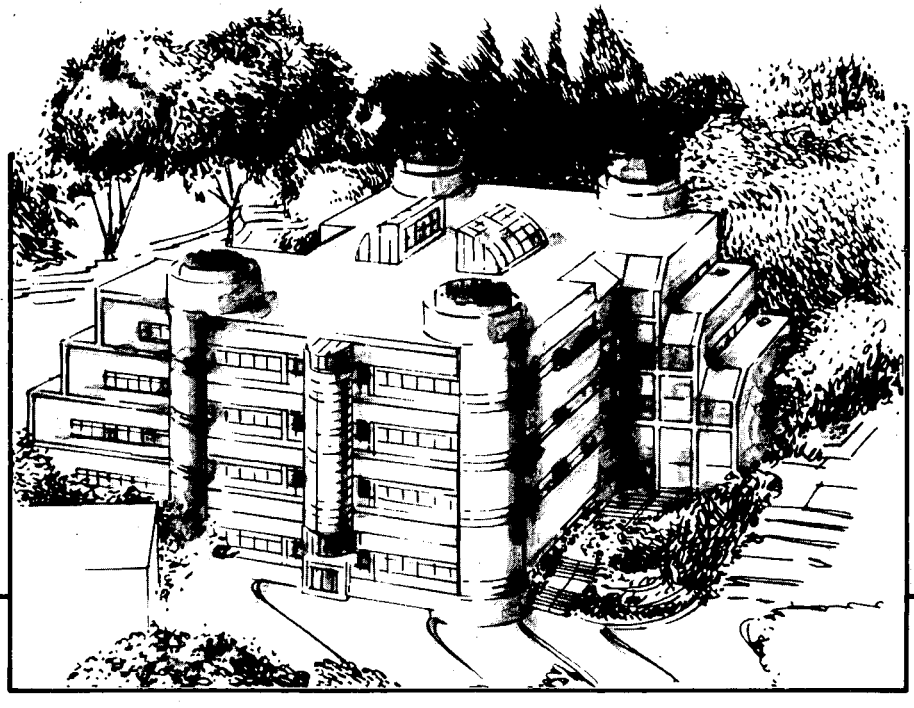

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ELECTRON SCATTERING BY NATIVE DEFECTS IN III-V NITRIDES AND THEIR ALLOYS

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ABSTRACT

We have calculated the electron mobilities in GaN and InN taking into consideration scattering by short range potentials, in addition to all standard scattering mechanisms. These potentials are produced by the native defects which are responsible for the high electron concentrations in nominally undoped nitrides. Comparison of the calculated mobilities with experimental data shows that scattering by short range potentials is the dominant mechanism limiting the electron mobilities in unintentionally doped nitrides with large electron concentrations. In the case of $Al_xGa_{1-x}N$ alloys, the reduction in the electron concentration due to the upward shift of the conduction band relative to the native defect level can account for the experimentally measured mobilities. Resonant scattering is shown to be important when the defect and Fermi levels are close in energy.

INTRODUCTION

Much research currently focuses on the growth of high quality epitaxial films of III-V nitrdes. Because of their wide direct bandgap, these materials are considered prime candidates for the manufacture of visible to ultraviolet optoelectronic devices [1] and the III-V compatible dielectrics [2]. In recent years there have been several reports on calculations of electron mobilities in III-V nitrides [3-5]. Those calculations were aimed at an assessment of the relative contributions of the standard scattering mechanisms and the establishment of the phonon mobility limits in these materials. Comparison of the calculations with experimental results was rather difficult as undoped GaN and InN very often exhibit large electron concentrations.

It has been argued before and there is an increasingly convincing body of evidence that the electrons found in nominally undoped nitrides originate from nitrogen vacancies with the first ionization level resonant with the conduction band [6,7]. It has been found that by controlling the crystal stoichiometry one can change the electron concentrations by many orders of magnitude with the highest concentrations exceeding 10^{20} cm^{-3}. The highly localized nature of the native donors raises the question on how the short range potential associated with the donors affects the electron mobilities and whether there is any difference in the electron mobilities in intentionally and unintentionally doped materials.

MOBILITIES IN BINARY III-V NITRIDES

Our calculations of the electron mobilities are based on a variational approach used previously to calculate mobilities in other III-V compounds [8]. We incorporate all standard scattering mechanisms; optical phonon, acoustic deformation potential, acoustic phonon piezoelectric and Coulombic ionized-impurity scattering. We also include the scattering arising from the short range potential of the native defects. This type of scattering has been previously considered in narrow gap semiconductors [9].

The total potential of an ionized and highly localized defect can be separated into two parts,

$$V(r) = V_{Coul}(r) + V_{sr}(r) \qquad (1)$$

where V_{coul} is the long range screened Coulomb potential and V_{sr} is the short range potential. Both potentials are localized on the same center. The electron scattering rate is proportional to the square matrix element of the potential (1) and consists of three terms; the standard Coulomb

term, a short range term proportional to the square of the matrix element $\langle S|V_{sr}|S\rangle$ and an interference term proportional to $\langle S|V_{sr}|S\rangle \langle S|V_{Coul}|S\rangle$, where $|S\rangle$ is the conduction band Bloch amplitude. Therefore, incorporation of the short range potential results in two additional terms in the total scattering rate,

$$\tau_{sr} = \frac{\hbar^3 \pi}{N m^* k A^2} \tag{2}$$

and

$$\tau_{int} = \frac{\hbar^3 \varepsilon_0 k}{N e^2 m^* A F_{int}} \tag{3}$$

where A is the matrix element of the short range potential, N is the concentration of native defects, k is the electron wavevector, m* is the effective mass in units of the free electron mass, and ε_0 is the dielectric constant.

The screening factor is

$$F_{int} = 4\left[1 - \frac{1}{\xi_0} \ln(1 + \xi_0)\right] \tag{4}$$

where $\xi_0 = (2k\lambda)^2$ and the screening length λ is [8]

$$\lambda = 1.72 \times 10^{-14} \frac{\varepsilon_0}{(m^*/m_0)^{3/2}\, T^{1/2}} \frac{1}{F_{-1/2}(x)} \tag{5}$$

where $F_{-1/2}(x)$ is the Fermi integral of -1/2 order. It is important to note the different dependence of the scattering rates on electron energy. For a highly degenerate electron gas with concentration n, $k \propto n^{1/3}$, $\lambda \propto n^{-1/6}$ and to a good approximation $F_{int} = 4$. Assuming that in the unintentionally doped samples the electron concentration is proportional to the defect concentration, one finds from Eqs. (2) and (3), that $1/\tau_{sr} \propto n^{4/3}$ and $1/\tau_{int} \propto n^{2/3}$. It can also be shown for scattering by the coulomb centers that $1/\tau_{Coul} \propto n^{1/3}$. Hence, the short range scattering is expected to play a more important role in samples with a high free carrier concentration.

The results of our calculations for unintentionally doped GaN along with the best experimental data found in the literature [10-13] can be seen in Fig. 1. Here we assume that the concentration of electrons is equal to the concentration of the native defects. Shown are the calculated mobilities assuming that the sources of the electrons are all extrinsic Coulombic impurities (dotted line) or are native defects with a short range potential (solid line). Also plotted are the individual contributions to the solid line mobility from the short range and interference terms. As one can see, the experimental mobilities at very high carrier concentrations show a sudden drop far below the dotted line values, which can be understood by the incorporation of scattering by short range potentials associated with highly localized native defects. Although the dotted line mobilities were calculated assuming zero compensation, it is easily demonstrated that even with compensating acceptors, the mobility at large carrier concentrations would not show the sudden drop present in the experimental data, as Coulomb scattering has a relatively weak dependence on the carrier concentration. Although not shown, experimental data for mobilities in GaN intentionally doped with Si or Ge show only the expected weak dependence on electron concentration [14-17], even at very high carrier concentrations. The material parameters used in the calculations are listed in Table 1. We find that a value of $A = 3.7 \times 10^{-34}$ erg cm^3 for the short range scattering strength is required to account for the experimental data. Assuming that the short range potential is restricted to a single

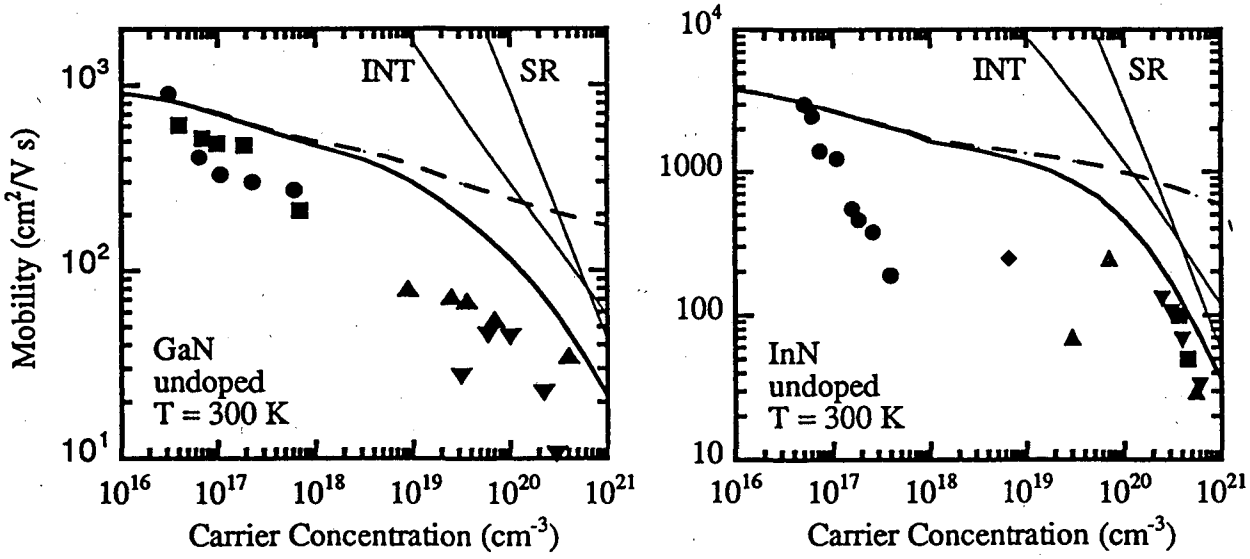
Table 1

	GaN	InN
density (g/cm^3)	6.1	6.81
ε_0	9.5	15.3
ε_∞	5.35	8.4
LO phonon energy (meV)	90.5	76
m^*/m_0 (at band minimum)	0.2	0.11
lattice parameter a_0 (Å)	4.52	4.98
acoustic phonon vel. (cm/s)	6.6×10^5	5.07×10^5
piezoelectric constant (V^2/dyn)	1326[a]	1326[a]
deformation potential (eV)	9.6	2.5
$\langle S\|V_{sr}\|S\rangle$	3.7×10^{-34}	2.5×10^{-34}

[a]Estimated from ref. 22. It is assumed that the value is similar for the two nitrides. Piezoelectric scattering is not an important mechanism in any concentration range.

unit cell this value corresponds to a potential well with a depth of about 10 eV. As there are no discussions of the magnitude of this parameter in the literature, the experimental mobilities were our only guide to estimating a value.

Another III-V compound that exhibits large concentrations of free electrons is InN. In as grown, undoped InN, electron concentrations are as high as 10^{21} cm^{-3}. It is generally accepted that in this case, the electrons also originate from highly localized native defects which have an energy level located well above the conduction band edge. One can therefore expect that scattering by short range potentials should play a significant role in this material as well.



Figures 1 and 2. Experimental (dots) and calculated (lines) mobilities in GaN and InN. The theoretical curves are calculated with (solid) and without (dashed) the short range potential. INT and SR show the contributions from the interference and short range terms, respectively.

Calculated room temperature electron mobilities in unintentionally doped InN are shown in Fig. 2 along with the best available experimental data [17-21]. Because of the relatively small energy gap of E_G =1.9 eV, at large carrier concentrations (>10^{19} cm^{-3}) the Fermi energy becomes comparable to the energy gap. In such cases it is necessary to incorporate the effects of nonparabolicity on the density of states effective mass. In a simple approximation, the energy dependent effective mass is given by,

$$m^* = m_0^* \left(1 + 2\frac{E}{E_G}\right) \qquad (6)$$

where m_0^* is the conduction band edge effective mass and E is the electron energy.

The results in Fig. 2 show that, as in GaN, the mobility is entirely determined by the short range and interference scattering at very high carrier concentrations. Although there is only a very limited amount of experimental data on electron mobilities in InN, it is quite clear that the strong concentration dependence observed at very high electron densities cannot be explained by Coulomb scattering. The rapid decrease of the mobility for n larger than 10^{20} cm^{-3} can be explained by scattering by native defects with the parameter A = 2.5×10^{-34} erg cm^3, which is close to it's value in GaN.

Unfortunately, there is no data available on InN which has been doped to such a high level. From the calculations presented in Fig. 2 one finds that at high electron concentrations the mobility in InN doped with hydrogenic donors should be at least one order of magnitude higher than in the unintentionally doped material. Therefore it is expected that doping with shallow hydrogenic donors should greatly improve the electrical characteristics of InN.

MOBILITIES IN THE ALLOYS OF III-V NITRIDES

In addition to the binary III-Nitrides, we have also examined mobilities in $Al_xGa_{1-x}N$. One noteworthy feature of the experimental mobility data in this material is that the electron mobilities remain relatively constant as a function of alloy composition [23,24]. In order to try to reproduce this trend, we introduce two more terms in our mobility calculations, alloy disorder [25], which is a well established scattering mechanism, and resonant scattering [26].

Figures 3A and 3B show the energies of various levels in $Al_xGa_{1-x}N$ as a function of Al content for two different defect concentrations. As the bandgap of AlN is greater than GaN, the conduction band minimum shifts upward with increasing Al fraction. The energy of the defect level remains relatively constant as it is localized. This decrease in energy of the defect level with respect to the conduction band leads to a "freeze out" of carriers originating from these defects. The calculations presented in Figs 3A and 3B include a downward shift of the conduction band edge resulting from electron-electron and electron-ion interaction [27]. As the electrons freeze out, the effect becomes smaller, leading to a superlinear dependence of the total shift on the alloy composition.Another effect we have considered is the influence of the carriers on the conduction band.

Resonant scattering becomes possible as the defect and Fermi levels move close to each other. At this point, conduction electrons may be scattered into temporarily bound states of the defect and vice versa. The overall effect of this process is to decrease the electron mobility [28]. This effect is particularly pronounced where the Fermi level and defect level coincide.

In order to take this effect into account, we introduce another scattering term into our calculations, making the assumption that the density of states of the defect level is not a delta function, but is broadened with a Lorentzian shape. In this case, the characteristic relaxation time for this process can be written as

$$\tau_{res} = \frac{N\, m^*\, k}{2\pi\hbar}\left[\frac{\Gamma^2}{(E_{def} - E)^2 + \Gamma^2}\right]^{-1} \qquad (6)$$

where E is the electron energy and Γ is the broadening of the defect level [29]. A value of 25 meV was adopted for Γ in these calculations.

The results of our calculations for alloys are shown in Figures 4A and 4B along with the corresponding experimental data. The general agreement between the two sets of data is quite good. The sudden decrease in the calculated mobility occurs where the Fermi and defect levels cross, suggesting that the experimentally measured dips are not due to experimental error or poor growth, but are in fact signatures of resonant scattering. We expect that this effect could also be seen if hydrostatic pressure were used to bring the defect level down in energy with respect to the conduction band. Such a measurement could be used to determine the pressure coefficients of the conduction band and defect level more accurately.

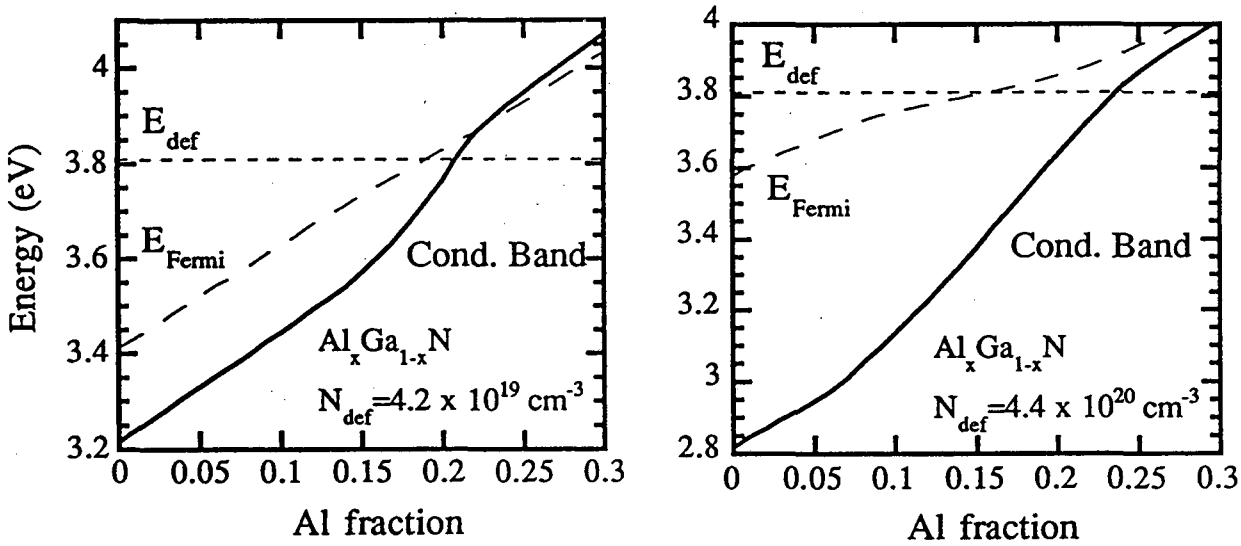


Figure 3A/B. Plot of energy levels v. Al content in $Al_xGa_{1-x}N$ for two defect concentrations showing Fermi and defect levels and conduction band.

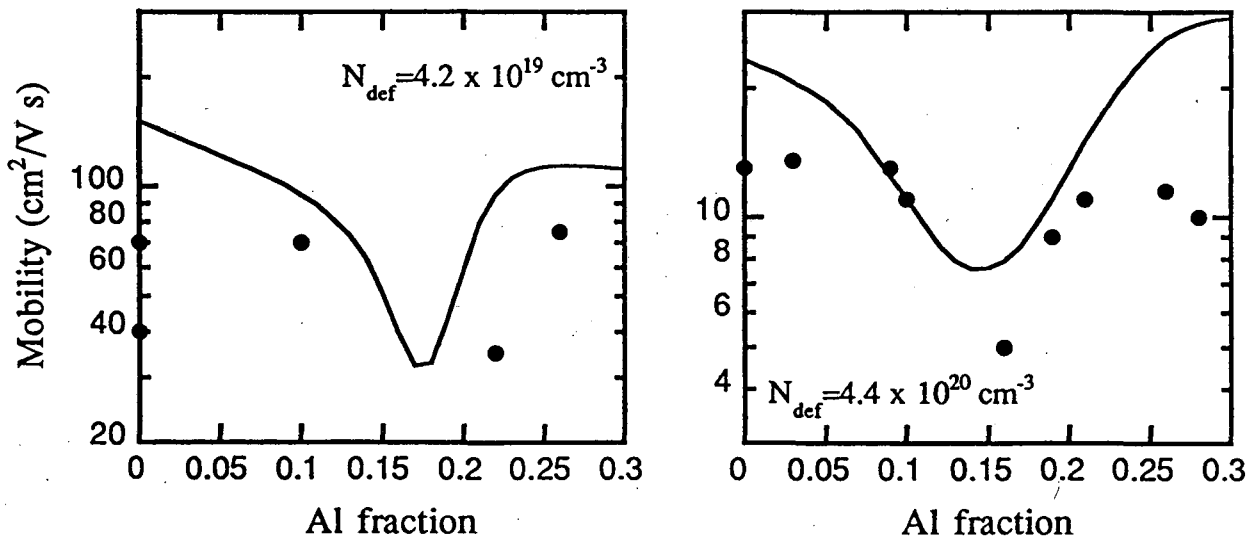


Figure 4A/B. Plot of experimental (dots) and theoretical (line) mobility in $Al_xGa_{1-x}N$ as a function of Al content for two defect concentrations.

CONCLUSIONS

We have presented the results of theoretical calculations of the electron mobility in GaN and InN. We have shown that scattering by the short range potential of highly localized native defects is responsible for the mobility drop observed at high electron concentrations in unintentionally doped materials and that resonant scattering can be seen by measuring mobilities in the case where the defect and Fermi levels are close in energy. The matrix element of the short range potential has been determined by comparison of the theoretical calculations with the experimental mobilities in unintentionally doped materials with high electron concentrations.

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