

# Hall mobilities in $\text{GaN}_x\text{As}_{1-x}$

Javier Olea<sup>\*1</sup>, Kin Man Yu<sup>\*\*2</sup>, Wladek Walukiewicz<sup>2</sup>, and Germán Gonzalez-Díaz<sup>1</sup>

<sup>1</sup> Dpto. de Física Aplicada III, Facultad de Ciencias Físicas, Universidad Complutense de Madrid, Madrid 28040, Spain

<sup>2</sup> Materials Sciences Division, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720-8197, USA

Received 3 October 2009, revised 11 December 2009, accepted 14 December 2009

Published online 12 May 2010

**Keywords** GaNAs, OMVPE, doping, Hall mobility, carrier scattering

\* Corresponding author: e-mail oleaariza@fis.ucm.es, Phone: +34 913 944 434, Fax: +34 913 945 196

\*\* e-mail kmyu@lbl.gov

In this work we report a systematic study of the electron and hole mobilities of  $\text{GaN}_x\text{As}_{1-x}$  alloys with different dopants (Zn, Te) and carrier concentrations ( $10^{17}$ – $10^{19} \text{ cm}^{-3}$ ). We found a very slight reduction of the hole mobility in p- $\text{GaN}_x\text{As}_{1-x}$  compared to p-GaAs, indicating that for small N contents ( $\sim 1.6\%$ ) the valence band is not affected by the N incorporation. In a striking contrast, incorporation of even small amounts of N leads to an abrupt reduction of the electron mobility in n- $\text{GaN}_x\text{As}_{1-x}$ .

We further show that the processes that limit the mobility in  $\text{GaN}_x\text{As}_{1-x}$  can be explained by the band broadening and the random field scatterings. Considering these two scattering mechanisms we calculated the dependence of electron mobilities on electron concentration as well as on N composition in  $\text{GaN}_x\text{As}_{1-x}$ . The calculations agree reasonably well with experiment data of maximum electron mobilities with alloy composition.

© 2010 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

**1 Introduction** Dilute nitride alloys have been studied for over a decade [1], due to their unusual physical properties and their technological potential for optoelectronic devices. These materials belong to the so-called highly mismatched alloys (HMAs), in which elements with very different electronegativity and/or size are alloyed to form a new class of semiconductors [2].  $\text{GaN}_x\text{As}_{1-x}$  with a small fraction of As replaced with N, is a very remarkable example of HMA. The higher electronegativity of N produces drastic changes in the band structure of GaAs, which influences its optical and electrical properties. Specifically, N interaction with the conduction band of GaAs leads to a reduction of the fundamental bandgap [3], an increase in the conduction band effective mass [4] and greatly improved the electrical activation of donors [5].

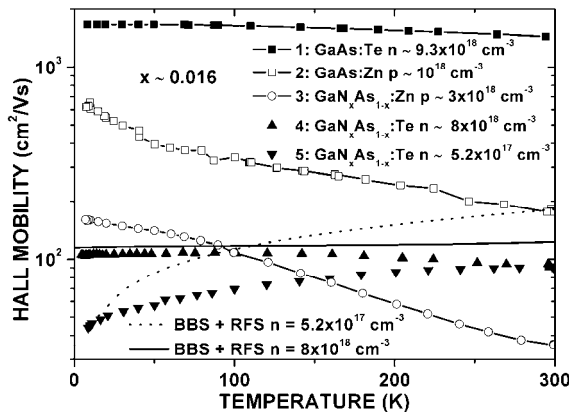
The salient feature of GaNAs alloys is the splitting of the conduction band due to the anticrossing interaction of the localized As states and the GaAs conduction band states. The splitting is described by the band anticrossing (BAC) model [6]. This model effectively predicts the properties of the alloy after the split, and describes the dispersion relation of the new bands,  $E_+(k)$  and  $E_-(k)$ . The resulting structure is typical of a multiband semiconductor, which can be used for high efficiency solar cells [7].

Despite years of extensive studies only a very limited effort has been directed towards understanding of the

transport properties of the GaNAs alloy system [8–15]. It has been shown that mobility in the  $\text{In}_y\text{Ga}_{1-y}\text{N}_x\text{As}_{1-x}$  is limited mainly by two scattering mechanisms: the band broadening scattering (BBS) and the random field scattering (RFS) [3]. The former is deduced from the BAC model, and the later is a consequence of the random arrangement of the N impurities in the GaAs lattice, which produces a smooth field that is the source of scattering [16]. The aim of this paper is to study the electron and hole mobilities in  $\text{GaN}_x\text{As}_{1-x}$ , and to propose a model based on these two mechanisms that can explain the mobility behavior with temperature, N concentration and carrier concentration.

**2 Experimental** Both p and n type  $\text{GaN}_x\text{As}_{1-x}$  thin films doped with Zn and Te, respectively were grown by organometallic vapour phase epitaxy (OMVPE) using Dimethylhydrazine (DMHz) at a growth temperature of 600 °C. N composition in these films was estimated to be  $\sim 1.6\%$  by x-ray diffraction and bandgap measured by photoreflectance. Hall effect measurements were performed in a homemade cryostat from liquid-He temperature to room temperature using the van der Pauw configuration.

| Report Documentation Page                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |                                    |                                     |                                                           | Form Approved<br>OMB No. 0704-0188                  |                                 |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------|-------------------------------------|-----------------------------------------------------------|-----------------------------------------------------|---------------------------------|
| Public reporting burden for the collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to a penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number. |                                    |                                     |                                                           |                                                     |                                 |
| 1. REPORT DATE<br><b>OCT 2009</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                    | 2. REPORT TYPE                      |                                                           | 3. DATES COVERED<br><b>00-00-2009 to 00-00-2009</b> |                                 |
| 4. TITLE AND SUBTITLE<br><b>Hall mobilities in GaN<sub>x</sub>As<sub>1-x</sub></b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |                                    |                                     |                                                           | 5a. CONTRACT NUMBER                                 |                                 |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                    |                                     |                                                           | 5b. GRANT NUMBER                                    |                                 |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                    |                                     |                                                           | 5c. PROGRAM ELEMENT NUMBER                          |                                 |
| 6. AUTHOR(S)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                    |                                     |                                                           | 5d. PROJECT NUMBER                                  |                                 |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                    |                                     |                                                           | 5e. TASK NUMBER                                     |                                 |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                    |                                     |                                                           | 5f. WORK UNIT NUMBER                                |                                 |
| 7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)<br><b>Lawrence Berkeley National Laboratory, Materials Sciences Division, 1 Cyclotron Road, Berkeley, CA, 94720-8197</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |                                    |                                     |                                                           | 8. PERFORMING ORGANIZATION REPORT NUMBER            |                                 |
| 9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                    |                                     |                                                           | 10. SPONSOR/MONITOR'S ACRONYM(S)                    |                                 |
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                    |                                     |                                                           | 11. SPONSOR/MONITOR'S REPORT NUMBER(S)              |                                 |
| 12. DISTRIBUTION/AVAILABILITY STATEMENT<br><b>Approved for public release; distribution unlimited</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |                                    |                                     |                                                           |                                                     |                                 |
| 13. SUPPLEMENTARY NOTES<br><b>See also ADM002356. Presented at the International Conference on Nitride Semiconductors (8th) (ICNS8) Held in Jeju, Korea on October 18-23, 2009. Sponsored by AOARD.</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |                                    |                                     |                                                           |                                                     |                                 |
| 14. ABSTRACT                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |                                    |                                     |                                                           |                                                     |                                 |
| 15. SUBJECT TERMS                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |                                    |                                     |                                                           |                                                     |                                 |
| 16. SECURITY CLASSIFICATION OF:                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |                                    |                                     | 17. LIMITATION OF ABSTRACT<br><b>Same as Report (SAR)</b> | 18. NUMBER OF PAGES<br><b>4</b>                     | 19a. NAME OF RESPONSIBLE PERSON |
| a. REPORT<br><b>unclassified</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       | b. ABSTRACT<br><b>unclassified</b> | c. THIS PAGE<br><b>unclassified</b> |                                                           |                                                     |                                 |



**Figure 1** Hall mobility vs. temperature of GaAs and GaN<sub>x</sub>As<sub>1-x</sub> samples. BBS+RFS model is applied for the Te doped GaN<sub>x</sub>As<sub>1-x</sub> samples with  $x = 0.016$ .

**3 Results and discussion** Figure 1 shows the Hall mobility measured for 5 representative samples. Mobilities of GaN<sub>x</sub>As<sub>1-x</sub> samples are always lower than mobilities of the GaAs samples of the same type. The slight reduction of the mobility in the p-type GaN<sub>x</sub>As<sub>1-x</sub> samples can be explained by the scattering produced by the N atoms, since for small N contents the valence band is not affected by alloying of GaAs with GaN [2, 3]. In the case of the n-type samples, the considerable decrease of the mobility is not only caused by this mechanism. Additional contribution to the reduction of the Hall mobility comes from a change of the dispersion relation  $E_c(k)$  and from a large increase of the electron effective mass [3]. It is also interesting to note that although sample 4 has more than 15 times higher carrier concentration than sample 5, they have very similar room temperature mobility. However it should be also noted that the temperature behavior of Hall mobility is completely different in these two samples. This indicates that different scattering mechanisms limit the electron mobility of GaN<sub>x</sub>As<sub>1-x</sub>, depending on the carrier concentration of the sample, the N concentration, and the temperature.

Initial estimates have shown that the traditional scattering mechanisms, such as alloy scattering [17], neutral impurity scattering [18] or deformation potential scattering [19], are negligible in n-GaN<sub>x</sub>As<sub>1-x</sub>. Only the ionized impurity scattering [20] should be considered for very high carrier concentration ( $n > 10^{19} \text{ cm}^{-3}$ ).

The BBS is dependent on the strength of the hybridization of the states in the  $E_c(k)$  band that could limit the lifetime of carriers, and it can be estimated through the BAC model. Details of this model is described in Ref. [2] and [3]. In this model the mobility can be expressed as:

$$\mu = \frac{e\tau(k_F)}{m_-(k_F)} \approx \frac{eh}{m_-(k_F)\Gamma_-(k_F)} \quad (1)$$

where  $e$  is the electron charge,  $\hbar$  is the reduced Planck constant,  $m_-$  is the mass of the carriers in the  $E_c(k)$  band,  $k_F$  is the Fermi surface wavevector and  $\Gamma_-$  is the broadening of the dispersion relations [3]. For the calculation of equation (1) we assumed a parabolic model for the GaAs conduction band, choosing for the conduction band minimum the Varshni empirical model and a linear behavior with temperature for the effective mass [21]. The prefactor for the energy broadening  $\beta$  [2] was treated as a fitting factor and a value of 0.3 was chosen, very close to the 0.22 estimated by Wu *et al.* for InGaAs [2].

To model the RFS, the onset of a smooth field has to be considered. Depending on the sign of the Fermi level, two different formulas are used [16]:

$$\mu = \frac{3\pi}{8} e \sqrt{\frac{E_F}{2m_-(k_F)\Psi_2}}, \quad E_F > 0 \quad (2)$$

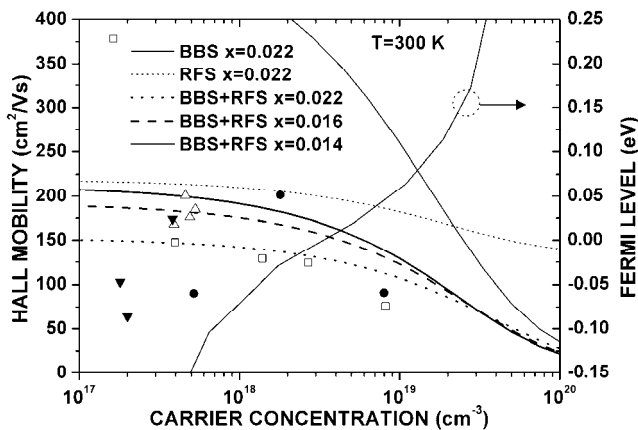
$$\mu = e \sqrt{\frac{\pi kT}{2m_-(k_F)\Psi_2}}, \quad E_F < 0 \quad (3)$$

where  $k$  is the Boltzmann constant,  $T$  is the absolute temperature and  $\Psi_2$  is the mean square of the gradient of the fluctuations of the potential energy of an electron in the random field. In the calculation of the Fermi level, integration converges in a small range of energy [2, 3]. Defining a cubic volume inside the lattice, where the standard deviation of N concentration can be estimated, one can use the BAC model to evaluate the magnitude of the variation of the field. Relating this variation to the average distance between N atoms, and multiplying by a constant fitting factor, we estimated  $\Psi_2$  to be in the range of  $10^4 \leq \Psi_2^{1/2} \leq 10^5 \text{ eV/cm}$  for a slow varying field [22]. Matthiessen's rule is used to calculate the combined effect of BBS and RFS.

Figure 1 includes the calculations for Hall mobility of samples 4 and 5 with varying temperature, using equation (1) to evaluate the BBS, and Eqs. (2) and (3) to estimate the RFS. As is seen in Fig. 1 the calculations well reproduce the magnitude as well as the temperature dependence of the mobility. The only difference between samples 4 and 5 is the carrier concentration, and that requires the use of equation (2) for sample 5, in which Fermi level is negative, and equation (3) for sample 4, in which Fermi level is positive. The BBS seems to dominate at higher electron concentration when the Fermi level is located closer to the N-level (see Fig. 2), whereas the RFS plays a more important role at low concentrations and lower temperatures, when the potential fluctuations are comparable to or larger than the average electron energy. In Ref. [15] temperature behavior of GaN<sub>x</sub>As<sub>1-x</sub> mobility is modeled, but this model does not account for the different temperature dependences presented in Fig. 1.

Figure 2 shows the calculated carrier concentration dependence of the mobility for different N concentrations, at

300 K. The trend is different from that reported by Shan *et al.* [3], but it is consistent with experimental results reported in the literature [11, 24, 26]. The saturation of the mobility at low carrier concentration has been previously reported in Ref. [11], but in this case the low carrier concentration mobility saturates at about an order of magnitude higher value. Also, the calculations presented in Ref. [8] for  $x=0.02$  give mobilities higher than our prediction.

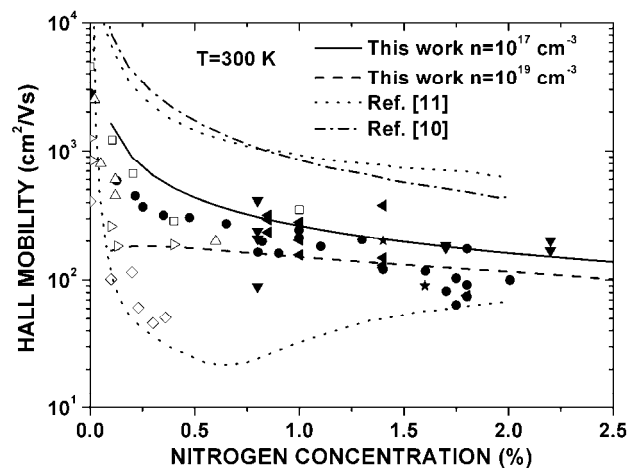


**Figure 2** Hall mobility as a function of carrier concentration. Experimental results ( $0.014 < x < 0.022$ ) from: ( $\square$ ) Ref. [11], ( $\blacktriangledown$ ) Ref. [24], ( $\triangle$ ) Ref. [26], ( $\bullet$ ) our measurements. Fermi level was calculated at room temperature for  $x=0.016$ .

Variation of Fermi level with carrier concentration for  $x=0.016$  is also plotted in Fig. 2. It is worth noting that equations (2) and (3) are only valid in the range  $|E_F| > kT$  [16], therefore, strictly speaking, at  $T=300$  K our model might not be valid in the carrier concentration range  $2 \times 10^{18}$ – $6 \times 10^{18} \text{ cm}^{-3}$ .

Finally, Fig. 3 shows results of the N concentration dependent mobility combining the BBS and RFS. All the experimental data points are either below or very close to our calculations, confirming the validity of the model. Calculations by Fahy and O'Reilly [10] and Vaughan and Ridley [11] are also shown in Fig. 3. Although the actual mobility values calculated using the different models differ significantly all of the calculations reproduce a much weaker dependence on the N concentration observed at high N contents. Similar behavior was also found previously in [14] and [15].

**4 Conclusions** Two different scattering mechanisms are proposed to explain the behavior of Hall mobility for n-type  $\text{GaN}_x\text{As}_{1-x}$ . We have found that band broadening scattering is dominant at high electron concentrations whereas random field scattering prevails at low electron concentrations and at lower temperatures. On the other hand, random field scattering is more important in the high N concentration range. These two processes describe reasonably well our experimental results and those reported in the literature.



**Figure 3** Hall mobility as a function of N concentration. ( $\blacktriangleleft$ ) Ref. [11], ( $\triangle$ ) Ref. [12], ( $\square$ ) Ref. [14], ( $\diamond$ ) Ref. [23], ( $\bullet$ ) Ref. [24], ( $\diamond$ ) Ref. [25], ( $\blacktriangledown$ ) Ref. [26], ( $\star$ ) our measurements.

**Acknowledgements** This work was made possible thanks to the FPI (Grant No. BES-2005-7063) of the Spanish Ministry of Education and Science and by U.C.M.-C.A.M. under Grant CCG07-UCM/TIC-2804. The work performed in LBNL was supported by the Director, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

## References

- [1] A. Erol (ed.), Physics of Dilute III-V Nitride Semiconductors and Materials System: Physics and Technology, (Springer-Verlag, Berlin/Heidelberg, 2008).
- [2] J. Wu, W. Shan, and W. Walukiewicz, *Semicond. Sci. Technol.* **17**, 860 (2002).
- [3] W. Shan et al., *J. Phys.: Condens. Matter* **16**, S3355 (2004).
- [4] C. Skierbiszewski et al., *Appl. Phys. Lett.* **76**, 2409 (2000).
- [5] K. M. Yu et al., *Appl. Phys. Lett.* **77**, 3607 (2000).
- [6] W. Shan et al., *Phys. Rev. Lett.* **82**, 1221 (1999).
- [7] K. M. Yu et al., *Phys. Status Solidi B* **241**, 660 (2004).
- [8] S. Fahy, A. Lindsay, H. Ouerdane, and E. P. O'Reilly, *Phys. Rev. B* **74**, 035203 (2006).
- [9] A. Hashimoto, T. Yamaguchi, T. Suzuki, and A. Yamamoto, *J. Cryst. Growth* **278**, 532 (2005).
- [10] S. Fahy and E. P. O'Reilly, *Appl. Phys. Lett.* **83**, 3731 (2003).
- [11] M. P. Vaughan and B. K. Ridley, *Phys. Rev. B* **75**, 195205 (2007).
- [12] R. Mouillet et al., *Solid State Commun.* **126**, 333 (2003).
- [13] S. Dhar, A. Mondal, and T. D. Das, *Semicond. Sci. Technol.* **23**, 015007 (2008).
- [14] A. Patané et al., *Appl. Phys. Lett.* **93**, 252106 (2008).
- [15] M. P. Vaughan and B. K. Ridley, *Phys. Rev. B* **72**, 075211 (2005).
- [16] P. G. Zhumatii, *Phys. Status Solidi B* **75**, 61 (1976).
- [17] L. Makowski and M. Glicksman, *J. Phys. Chem. Solids* **34**, 487 (1973).

- [18] C. Erginsoy, Phys. Rev. **79**, 1013 (1950).
- [19] J. Bardeen and W. Shockley, Phys. Rev. **80**, 72 (1950).
- [20] E. Conwell and V. F. Weisskopf, Phys. Rev. **77**, 388 (1950).
- [21] J. S. Blackmore, J. Appl. Phys. **53**, R123 (1982).
- [22] V. L. Bonch-Bruевич, Phys. Status Solidi **42**, 35 (1970).
- [23] D. L. Young, J. F. Geisz, and T. J. Coutts, Appl. Phys. Lett. **82**, 1236 (2003).
- [24] M. Reason et al., J. Appl. Phys. **102**, 103710 (2007).
- [25] J. Ibáñez et al., J. Appl. Phys. **103**, 103528 (2008).
- [26] F. Ishikawa et al., Appl. Phys. Lett. **87**, 262112 (2005).