Reflection anisotropy spectroscopy study of the near-surface electric fields in undoped, *n*- and *p*-doped low-temperature grown GaAs (001)

Todd Holden,* W. D. Sun, and Fred H. Pollak†
Physics Department and New York State Center for Advanced Technology in Ultrafast Photonic Materials and Applications, Brooklyn College of the City University of New York, Brooklyn, New York 11210

J. L. Freeouf
Interface Studies, Inc., Katonah, New York 10536

D. McInturff and J. M. Woodall
School of Electrical and Computer Engineering and NSF MRSEC for Technology Enabling Heterostructure Materials, Purdue University, West Lafayette, Indiana 47907

(Received 8 April 1998)

We have evaluated the effective surface electric fields, effective depletion widths, and the sign (*n*-type/upward band bending) of the near-surface electric fields in undoped as well as *n*-(5×10^{18} cm^{-3}) and *p*-(5×10^{18} cm^{-3} and 2×10^{19} cm^{-3}) doped low-temperature grown (LTG) GaAs (001) using the optical method of reflection-anisotropy (RA) spectroscopy in the vicinity of the spin-orbit split E_1, $E_1+\Delta_1$ optical features. Even for the highest *p* doping the surface band bending is still *n* type, indicating the strong influence of the large donor trap densities. Our results are in good agreement with a self-consistent Poisson's calculation of the near-surface electric fields assuming deep donor (1×10^{20} cm^{-3}) and acceptor (1×10^{19} cm^{-3}) trap densities and midgap surface Fermi-level pinning. This experiment provides valuable information about the defect density and position in LTG:GaAs. Our results will be compared to the recent RA spectroscopy experiment and interpretation of Chen *et al.* [Phys. Rev. B **55**, R7379 (1997)]. [S0163-1829(98)00536-0]

Low-temperature grown (LTG) GaAs, i.e., layers grown by molecular beam epitaxy (MBE) at substrate temperatures between 250–300 °C, possess a number of interesting electronic properties associated with the excess arsenic concentration incorporated during growth.[1] In as-grown LTG:GaAs material, the excess arsenic results in a large concentration of point defects (1×10^{20} cm^{-3}), due primarily to arsenic antisite defects. The pinning of the Fermi level near midgap in this material is generally associated with the point defects.[2,3] Also, the stability of LTG:GaAs against oxidation in air has recently been demonstrated using scanning tunneling microscopy.[4]

LTG:GaAs has been employed in a number of important applications.[1] First, when LTG:GaAs is annealed at temperatures between 600–900 °C the excess As in the form of antisite defects coalesces into As precipitates, and, hence, forms an elemental As phase of As clusters. These precipitates behave as buried Schottky barriers. As such, they exhibit 0.7 eV Schottky barrier heights and act as recombination centers for excess carriers. This property has resulted in realization of state-of-the-art high speed photodetector devices, with responsivities of nearly 0.1 A/W and cut-off frequencies of 40 GHz. This material has been shown to have useful nonlinear optical properties. Also, in the unannealed state, LTG:GaAs has been used to form excellent nonalloyed ohmic contacts when used in tandem with a thin layer of n^{++} GaAs.

In order to gain more information about the nature of the surface and associated electric fields in this material we have performed a reflection anisotropy (RA) spectroscopy[5–15] investigation of undoped as well as *n*- and *p*-doped LTG:GaAs (001). It has been demonstrated that RA spectroscopy can be employed to determine the sign and magnitude of near-surface electric fields in zinc-blende-type semiconductors. The results of our experiment have enabled us to evaluate (a) an effective depletion width of $\leqslant$20–22 Å and (b) the nature of the near-surface electric field, i.e., *n*-type (upward band-bending). The first result has been obtained by a comparison of the experimental data with a self-consistent Poisson's calculation based on the properties of the defects and surface Fermi level pinning in this material.

Sample 2 consisted of a not-intentionally doped (NID) LTG:GaAs film grown on a semi-insulating GaAs (001) substrate in a Gen II molecular beam epitaxy system. A 2000 Å thick buffer layer was grown at 580 °C prior to lowering the growth temperature to grow the LTG layer. A 5000-Å-thick LTG layer was grown at a substrate temperature of 250 °C as measured by a thermocouple. At this temperature the excess arsenic concentration is between 1 and 1.5%. The layers were grown at a rate of 1 μm/hr with As_2. Samples 1, 3, and 4 were grown under similar conditions, but were either *n*-doped at 5×10^{18} cm^{-3} (sample 1), or *p*-doped at levels of 5×10^{18} cm^{-3} (sample 3), and 2×10^{19} cm^{-3} (sample 4).

RA spectroscopy measures the polarization anisotropy of light linearly polarized along the [110] and [1$\bar{1}$0] principal axes in the plane of the (001) surface of zincblende-type semiconductors. RA spectroscopy can be employed to gain information about the sign and magnitude of near-surface electric fields in these semiconductors from the anisotropy produced by the linear electro-optic (LEO) effect in the vicinity of the spin-orbit split E_1, $E_1+\Delta_1$ optical features. For example, it has been shown that for a conventional space charge region (SCR), i.e., linear variation of the electric field with distance from the surface, the RA spectroscopy signal is

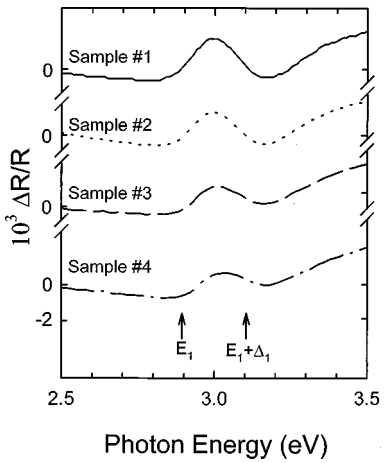

FIG. 1. RA spectra of sample 1 (solid line), sample 2 (dotted line), sample 3 (dashed line), and sample 4 (dot-dashed line). The positions of the E_1, $E_1+\Delta_1$ features are denoted by arrows at the bottom of the figure.

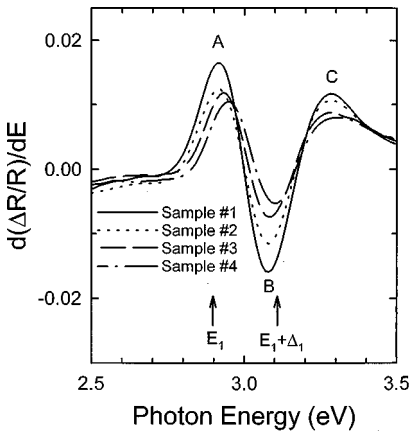

FIG. 2. $d(\Delta R/R)/dE$ spectra of sample 1 (solid line), sample 2 (dotted line), sample 3 (dashed line), and sample 4 (dot-dashed line). The positions of the E_1, $E_1+\Delta_1$ features are denoted by arrows at the bottom of the figure.

a direct measure of the surface electric field if the width of the SCR is much larger than the penetration depth of the light.[7] Reflection anisotropy spectroscopy experiments have been used to study the surface electric fields in *n*- and *p*-doped GaAs (001),[6,7,11] ZnSe (001),[8,11] and InGaAs/InP (001),[12] as well as InSb (110) (Ref. 9) and GaAs (110).[10] Paget *et al.* have used this method to investigate sulfur-passivated GaAs (001).[13] More recently, this method has been used to investigate the properties of undoped LTG:GaAs[14,15]

In addition to the LEO effect there may also be a background signal due to any improper alignment of the modulator and analyzer. Since it is the LEO effect that provides the information of interest, we would like to eliminate the influence of the background term. We define $(\Delta R/R)_1$ as:

$$(\Delta R/R)_1=(R_{[110]}-R_{[\bar{1}10]})/(R_{[110]}+R_{[\bar{1}10]}), \qquad (1a)$$

where $R_{[110]}$ and $R_{[\bar{1}10]}$ are the reflectivities for light polarized along the [110] and [110] directions, respectively. On the other hand the signal $(\Delta R/R)_2$ is

$$(\Delta R/R)_2=(R_{[\bar{1}10]}-R_{[\bar{1}\bar{1}0]})/(R_{[\bar{1}10]}+R_{[\bar{1}\bar{1}0]}). \qquad (1b)$$

The RA spectrum of interest $(\Delta R/R)$ is then obtained by taking the difference between these two signals, i.e., $\Delta R/R=(\Delta R/R)_1-(\Delta R/R)_2$ to eliminate any background terms.

Plotted in Fig. 1 by the solid, dotted, dashed, and dot-dashed curves are the RA spectra of samples 1–4, respectively, in the range 2.5–3.5 eV. The positions of the E_1 (2.88 eV) and $E_1+\Delta_1$ (3.11 eV) transitions[16] are denoted by arrows at the bottom of the figure. It can be seen that the phases of all the samples are the same and correspond to an *n*-type (upward) band bending.

In order to more accurately evaluate the amplitude of the LEO effect in the vicinity of the E_1, $E_1+\Delta_1$ features we have taken the numerical derivative with respect to photon energy of the spectra [designated as $d(\Delta R/R)/dE$] of the data. These results, which exhibit three extrema (*A*, *B*, and *C*), are shown in Fig. 2 for sample 1 (solid line), sample 2 (dashed line), sample 3 (dotted line), and sample 4 (dot-dashed line). As a measure of the amplitude of the LEO effect we have evaluated:

$$\frac{|d(\Delta R/R)/dE|_{AB}+|d(\Delta R/R)/dE|_{BC}}{2}. \qquad (2)$$

The ratios of the amplitude of this signal for samples 1, 2, 3, and 4 are 1.26:1.00:0.80:0.68, respectively.

In a previous investigation[14] we have calibrated the magnitude of the RA spectroscopy signal and found an effective surface electric field $\mathcal{E}_{\rm eff}=220$ kV/cm in the NID LTG:GaAs material. As discussed in Ref. 14, in contrast to previous experiments on semiconductors with a conventional SCR, in LTG:GaAs material the RA spectroscopy does not measure the surface electric field. The values of $\mathcal{E}_{\rm eff}$ for samples 1, 3, and 4 as well as sample 2 are listed in Table I.

It has been shown that[7]

$$\frac{\Delta R}{R}=\mathrm{Re}\left\{\frac{\langle\Delta\epsilon\rangle}{\sqrt{\epsilon}(\epsilon-1)}\right\}, \qquad (3a)$$

$$\langle\Delta\epsilon\rangle=2i\kappa_L\int_0^\infty e^{2i\kappa_L z}\Delta\epsilon(z)dz, \qquad (3b)$$

where $\Delta\epsilon(z)$ is the perturbation of the unperturbed dielectric function due to the electric field and $\kappa_L(=\kappa_{r,L}+i\kappa_{i,L})$ is the unperturbed complex propagation vector of the light. For the LEO effect $\Delta\epsilon(z)\propto\mathcal{E}(z)$. At 3.0 eV for GaAs (Ref. 17) the propagation vector $\kappa_L=(6.85+i2.96)\times10^{-3}$, in units of Å^{-1}.

In order to evaluate $\mathcal{E}(z)$ we have performed a self-consistent Poisson's calculation[18] assuming (a) a donor trap density ($N_{\rm TD}$) of 1×10^{20} cm^{-3} having a Gaussian distribution of states with width $\sigma(=0.2$ eV), the peak of the Gaussian distribution occurring 0.45 eV below the conduction band, (b) an acceptor trap density ($N_{\rm TA}$) of 1×10^{19} cm^{-3} having a Gaussian distribution of states with width σ $(=0.2$ eV), the peak of the Gaussian distribution occurring 0.45 eV above the valence band, and (c) midgap surface Fermi level pinning.[1] Shown in Fig. 3 by the solid, dotted,

TABLE I. Doping levels $\mathcal{E}_{\text{eff}}$ (experiment and simulation) $\mathcal{E}(0)$, γ, and $1/\alpha_{\text{eff}}$ for the four LTG-GaAs samples.

Sample	Doping (10^{18} cm^{-3})	$\mathcal{E}_{\text{eff}}$ (kV/cm) Experiment (a)	$\mathcal{E}_{\text{eff}}$ (kV/cm) Simulation (a)	$\mathcal{E}(0)$ (kV/cm)	γ	$1/\alpha_{\text{eff}}$ (Å)
1	5 (n type)	277	276	1550	17.8	22.2
2	NID	220	230	1380	16.6	20.8
3	5 (p type)	176	200	1240	16.1	20.4
4	20 (p type)	150	135	850	16.1	20.0

[a] n-type band bending.

dashed, and dot-dashed curves are the results of this calculation for $\mathcal{E}(z)$ for samples 1–4, respectively. Note that even for the two p-type samples (i.e., samples 3 and 4), the band-bending is still n type. Also, the electric field does not vary linearly with position from the surface, as would be the case for a fully depleted SCR. The values of the surface field $\mathcal{E}(0)$ are listed in Table I.

We have numerically integrated Eq. (3b) with the computed $\mathcal{E}(z)$ of Fig. 3 and find that $\text{Re}\langle\Delta\epsilon\rangle \propto \gamma\mathcal{E}(0)$, the values of γ being listed in Table I. This procedure also yields the effective surface electric fields that are given in Table I. These values are in good agreement with our experimental results.

Although the dependence of the electric field on position from the surface does not have a simple analytical behavior, it is close to an exponential form (see Fig. 3). Thus, an effective depletion width can be evaluated if we assume that:

$$\mathcal{E}(z) = \mathcal{E}(0)e^{-\alpha_{\text{eff}}z}, \tag{4}$$

where the quantity $1/\alpha_{\text{eff}}$ can be considered as the effective depletion width. If Eqs. (3b) and (4) are used to yield $\mathcal{E} = \gamma\mathcal{E}(0)$, we find the values of $1/\alpha_{\text{eff}}$ listed in Table I. Note that all of these correspond to an effective depletion width of about 20–22 Å. The above simple analytical function probably underestimates α_{eff}. Therefore, we conclude that the effective depletion width $\leqslant$20–22 Å.

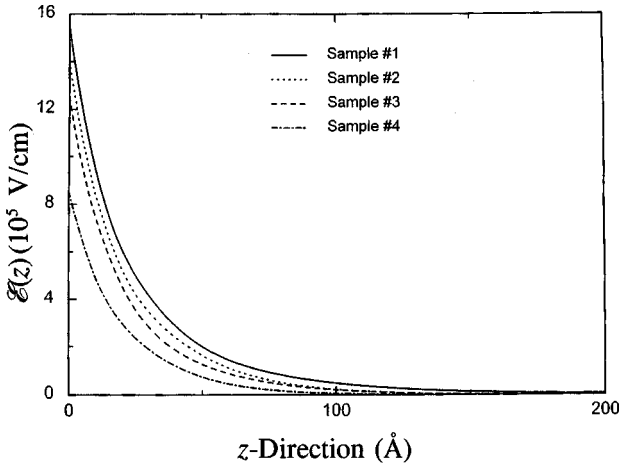

FIG. 3. Self-consistent Poisson's calculation of the field distribution $\mathcal{E}(z)$ as a function of position from the surface for LTG:GaAs sample 1 (solid line), sample 2 (dotted line), sample 3 (dashed line), and sample 4 (dot-dashed line).

It should be noted that our results for the simulation of the NID sample are somewhat different from those in Ref. 14 since in this work we have included N_{TA}.

Chen *et al.* also have recently reported a RA spectroscopy study of LTG:GaAs (001), including the effects of post growth annealing.[15] These authors conclude that the built-in potential (V_{bi}) for the unannealed material is about 0.1 V (relative to the conduction band), where $V_{\text{bi}} = \int \xi(z)dz$. From Eq. (4) we find for our undoped material $V_{\text{bi}} \approx 0.28$ V. However, Ref. 15 erroneously states that all the donor defects are ionized. Our result is consistent with a bulk Fermi level $\approx$0.45 V below the conduction band (as reported in Ref. 20 and also deduced from our simulation) and midgap surface Fermi-level pinning.

In conclusion, we have used RA spectroscopy at 300 K to evaluate the sign and magnitude of the near-surface electric field in NID, n-type and p-type LTG:GaAs (001). We also have performed a self-consistent Poisson's calculation to determine $\mathcal{E}(z)$. In contrast to a conventional SCR, in our material the field $\mathcal{E}(z)$ does not vary linearly with position. There is good agreement between our experimental determined effective near-surface electric fields and the calculation (midgap surface Fermi level pinning), yielding an effective depletion width $\leqslant$20–22 Å. Even for the two p-type samples the band-bending is still n-type, as a consequence of the large number of donorlike defects. We have compared our results and interpretation with the RA spectroscopy study of Ref. 15. Finally, since a 20–50 Å layer of LTG:GaAs is used in tandem with an n^{++} thin space charge layer of ''normal'' GaAs for nonalloyed ohmic contacts,[19] the design of this contact layer should be revisited now that there is evidence for midgap surface Fermi level pinning effects in LTG:GaAs.

Note added in proof. We also have recently performed RA spectroscopy from p-LTG:GaAs with an intended doping level of 2×10^{20} cm^{-3} (Ref. 21). It was found that the band bending was still n type, although nearly flat. Agreement between experiment and simulation was obtained by assuming that only 4×10^{19} cm^{-3} of the p dopants were electrically active.

T.H., W.D.S., and F.H.P. acknowledge support by the U.S. Army Research Office Contract No. DAAHO4-94-G-0153, National Science Foundation Grant No. DMR-9414209, PSC/BHE Grant No. 666424, and the New York State Science and Technology Foundation through its Centers for Advanced Technology program. D.M. and J.M.W. were supported in part by NSF-MRSEC Grant No. DMR-9400415.

*Also at the Graduate School and University Center of the City University of New York, New York, NY 10036.

†Also at the Graduate School and University Center of the City University of New York, New York, NY 10036. Electronic address: FHPBC@CUNYVM.CUNY.EDU

[1] See, for example, M. R. Melloch, J. M. Woodall, E. S. Harmon, N. Otsuka, F. H. Pollak, and D. D. Nolte, *Annual Review of Materials Science*, edited by B. W. Wessels, E. N. Kaufman, J. A. Giordmaine, and J. B. Wachtman, Jr. (Palo Alto, CA, Annual Reviews, 1995), Vol. **25**, p. 547, and references therein.

[2] R. M. Feenstra, J. M. Woodall, and G. D. Pettit, Phys. Rev. Lett. **71**, 1176 (1993).

[3] R. M. Feenstra, A. Vaterlaus, J. M. Woodall, and G. D. Pettit, Appl. Phys. Lett. **63**, 2528 (1993).

[4] S. Hong, R. Reifenberger, D. B. Janes, D. McInturff, and J. M. Woodall, Appl. Phys. Lett. **68**, 2258 (1996).

[5] See, for example, D. E. Aspnes, Mater. Res. Soc. Symp. Proc. **324**, 3 (1994); W. Richter, Philos. Trans. R. Soc. London, Ser. A **344**, 453 (1993); O. Acher, S. M. Koch, F. Omnes, M. Defour, M. Razeghi, and B. Drévillon, J. Appl. Phys. **68**, 3564 (1990).

[6] S. E. Acosta-Ortiz and A. Lastraz-Martinez, Phys. Rev. B **40**, 1426 (1989); also *Proceedings of the Society of Photo-optic Instrumentation Engineers*, edited by F. H. Pollak, M. Cardona, and D. E. Aspnes (SPIE, Bellingham, 1990), Vol. 1286, p. 31.

[7] H. Tanaka, E. Colas, I. Kamiya, D. E. Aspnes, and R. Bhat, Appl. Phys. Lett. **59**, 3443 (1991).

[8] H. H. Farrell, M. C. Tamargo, T. J. Gmitter, A. L. Weaver, and D. E. Aspnes, J. Appl. Phys. **70**, 1033 (1991).

[9] K. C. Rose, S. J. Morris, D. I. Westwood, D. A. Woolf, R. H. Williams, and W. Richter, Appl. Phys. Lett. **66**, 1930 (1995).

[10] Z. Yang, G. K. Wong, I. K. Sou, and Y. H. Yeung, Appl. Phys. Lett. **66**, 2235 (1995).

[11] C. C. Kim and S. Sivananthan, Mater. Res. Soc. Symp. Proc. **406**, 319 (1996).

[12] M. Leibovitch, P. Ram, L. Malikova, F. H. Pollak, J. L. Freeouf, L. Kronik, B. Mishori, Y. Shapira, A. R. Clawson, and C. M. Hanson, J. Vac. Sci. Technol. B **14**, 3089 (1996).

[13] D. Paget, J. E. Bonner, V. L. Berkovits, P. Chiaradia, and J. Avila, Phys. Rev. B **53**, 4604 (1996).

[14] T. Holden, F. H. Pollak, J. L. Freeouf, D. McInturff, J. L. Gray, M. Lundstrom, and J. M. Woodall, Appl. Phys. Lett. **70**, 1107 (1997).

[15] Y. H. Chen, Z. Yang, R. G. Li, Y. Q. Wang, and Z. G. Wang, Phys. Rev. B **55**, R7379 (1997).

[16] P. Lautenschlager, M. Garriga, S. Logothetidis, and M. Cardona, Phys. Rev. B **35**, 9174 (1987).

[17] D. E. Aspnes and A. A. Studna, Phys. Rev. B **27**, 985 (1983).

[18] Silvaco Data Systems, Santa Clara, CA 94054.

[19] M. P. Patkar, T. P. Chin, J. M. Woodall, M. S. Lundstrom, and M. R. Melloch, Appl. Phys. Lett. **66**, 1412 (1995).

[20] H. Shen and M. Dutta, J. Appl. Phys. **78**, 2151 (1995).

[21] T. Holden, W. D. Sun, F. H. Pollak, J. L. Freeouf, D. McInturff, M. R. Melloch, and J. M. Woodall, Proceedings of the 24th International Conference on the Physics of Semiconductors, Jerusalem, 1988, edited by D. Gershoni (World Scientific, Singapore, in press).