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Reflection anisotropy spectroscopy study of the near surface electric field in low-temperature grown GaAs (001)

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We have evaluated an ''effective depletion width'' of ⩽45 Å and the sign (n-type/upward band bending) of the near surface electric field in low-temperature grown GaAs (001) using the optical method of reflection anisotropy spectroscopy in the vicinity of the spin-orbit split E_1, $E_1+\Delta_1$ optical features. Our results provide evidence that surface Fermi level pinning occurs for air exposed (001) surfaces of undoped low temperature grown GaAs. [S0003-6951(97)00509-3]

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}) are 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]

Although much is known about the properties of both bulk and (110) UHV cleaved surfaces of LTG:GaAs,[1–3] there is little knowledge about the electronic properties of air-exposed (001) LTG:GaAs. Specifically, since the (001) LTG:GaAs surface is stable against oxidation,[4] it might be suspected that the Fermi level pinning associated with air-exposed surfaces of ''normal'' temperature grown GaAs, in which oxidation results in excess elemental As, should not occur for LTG:GaAs surfaces. Therefore, 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 spectroscopy (RAS)[5–12] investigation of LTG:GaAs (001) (designated sample No. 1) at 300 K. For comparison purposes, we also have studied an n-type sample (001) with a uniform surface field (sample No. 2) and n- and p-type (001) material (sample Nos. 3 and 4, respectively) with space-charge surface fields. Reflection anisotropy spectroscopy measures the polarization anisotropy of light linearly polarized along the [110] and $[\bar{1}10]$ principal axes in the plane of the (001) surface of zincblende-type semiconductors. It has been demonstrated that RAS can be employed to determine the sign and magnitude of near surface electric fields in zincblende-type semiconductors.[5–13] The results of our experiment have enabled us to evaluate (a) an ''effective depletion width'' of ⩽45 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[14] based on the properties of the defects and surface Fermi level pinning in this material.

Sample No. 1 consisted of a 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 percent. The layers were grown at a rate of 1 μm/h with As_2 and were undoped. Sample No. 2 consisted of 1000 Å of undoped GaAs fabricated on an n-type ($Si=2\times10^{18}$ cm^{-3}) buffer, 1 μm thick, on an n^+ (001) substrate. It has been shown that such a configuration has a uniform electric field in the undoped region due to Fermi level pinning at the surface.[15] The magnitude of this electric field (6.5×10^4 V/cm) was evaluated from the observed Franz–Keldysh oscillations (FKOs) using photoreflectance.[15] Sample Nos. 3 and 4 consisted of 0.5 μm 1×10^{18} cm^{-3} Si or Be doped layers on n^+ or p^+ substrates, respectively.

In addition to the linear electro-optic effect, there may also be a background signal which should be eliminated. We define $(\Delta R/R)_1$ as

$$(\Delta R/R)_1=(R_{[110]}-R_{[\bar{1}\bar{1}0]})/(R_{[110]}+R_{[\bar{1}\bar{1}0]}), \qquad (1a)$$

where $R_{[110]}$ and $R_{[\bar{1}10]}$ are the reflectivities for light polarized along the [110] and $[\bar{1}10]$ directions, respectively. 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 RAS 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.

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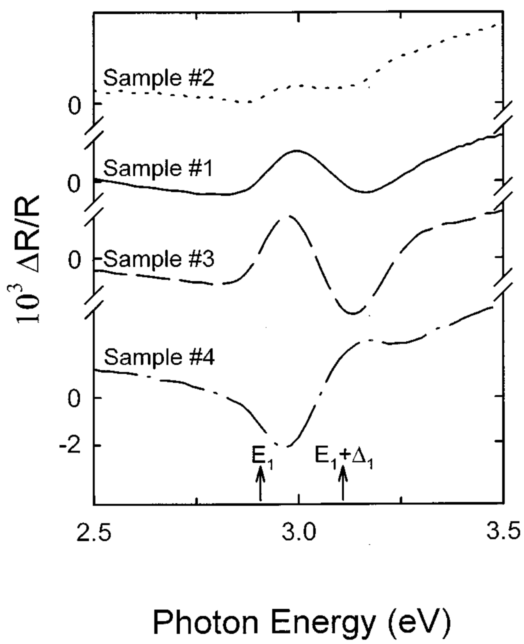

FIG. 1. RAS spectra of sample Nos. 1 (solid line), 2 (dotted line), 3 (dashed line), and 4 (dot-dashed line). The positions of the E_1, $E_1+\Delta_1$ features are denoted by arrows at the bottom of the figure.

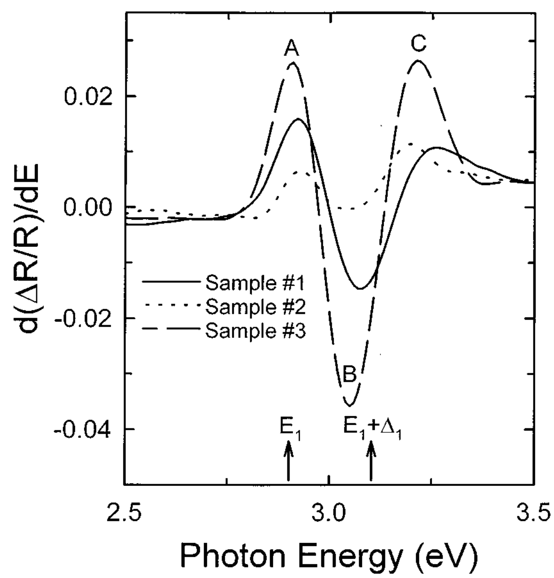

FIG. 2. $d(\Delta R/R)/dE$ spectra of sample Nos. 1 (solid line), 2 (dotted line), and 3 (dashed line). The positions of the E_1, $E_1+\Delta_1$ features are denoted by arrows at the bottom of the figure.

Plotted in Fig. 1 by the solid, dotted, dashed, and dot-dashed curves are the RAS spectra of sample Nos. 1–4, respectively, in the range of 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 sample Nos. 1–3 are opposite to that of sample No. 4. Thus the band bending of the LTG:GaAs material (sample No. 1) is clearly n type (upward band bending). Also the amplitude of the RAS signal for the LTG:GaAs material lies between that of sample Nos. 2 and 3.

In order to more accurately evaluate the amplitude of the linear electro-optic 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 LTG:GaAs (solid line) and sample Nos. 2 (dotted line) and 3 (dashed line). These results, which exhibit three extrema (A, B, and C), are shown in Fig. 2. As a measure of the amplitude of the linear electro-optic effect, we have evaluated

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

The ratios of the amplitude of this signal for sample Nos. 1, 2, and 3 are 2.9:1:6, respectively.

Because of the high doping level in sample No. 3, it was not possible to observe FKOs.[15] Therefore, for conventional SCR sample number 3 (with width of SCR≫penetration depth of the light), the surface electric field ($E_s=4.6\times10^5$ V/cm) has been evaluated from the relation[17]

$$E_s=[(2qN_D/\kappa_0\epsilon_0)(V_{F,s}^c-V_{F,b}^c-kT/q)]^{1/2}, \tag{3}$$

where N_D is the donor concentration (1×10^{18} cm^{-3}), ϵ_0 is the permittivity of free space, κ_0 (=13) is the static dielectric constant, and $V_{F,s}^c$ and $V_{F,b}^c$ are the surface and bulk Fermi levels (relative to the conduction band edge), respectively. It is well known that in as-grown n-type GaAs the Fermi level is pinned midgap so that $V_{F,s}^c=0.71$ V. For $N_D=1\times10^{18}$ cm^{-3}, $V_{F,b}^c$ lies 0.075 eV above the conduction band edge.

From a linear interpolation between the fields of sample Nos. 2 and 3, we find an ‘‘effective near surface electric field’’ $E_e=2.2\times10^5$ V/cm in the LTG:GaAs material. In contrast to previous experiments on semiconductors with a SCR, in this material, the RAS does not measure the surface electric field.

It has been shown that[7]

$$\frac{\Delta R}{R}=Re\left\{\frac{\langle\Delta\epsilon\rangle}{\sqrt{\epsilon}(\epsilon-1)}\right\}, \tag{4a}$$

$$\langle\Delta\epsilon\rangle=2i\kappa_L\int_0^\infty e^{2i\kappa_L z}\Delta\epsilon(z)dz, \tag{4b}$$

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 linear electro-optic effect $\langle\Delta\epsilon\rangle\propto E(z)$. At 3.0 eV for GaAs,[18] the propagation vector $\kappa_L=(6.85+i2.96)\times10^{-3}$, in units of Å^{-1}.

In order to evaluate $E(z)$, we have performed a self-consistent Poisson's calculation[14] assuming (a) a trap density (N_T) 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 0.25 eV below the intrinsic Fermi level, and (b) midgap surface Fermi level pinning.[1] Shown in Figs. 3(a) and 3(b) are the results of this calculation for the energy bands (solid lines) and $E(z)$, respectively. In Fig. 3(a), the dashed line is the Fermi level due to the donor states while the dotted line is the intrinsic Fermi level. In the bulk, the Fermi level lies about 0.3 eV below the conduction band edge, in agreement with Ref. 1. Note that in Fig. 3(b), the electric field does not vary linearly with position from the surface and that $E_s=4.5\times10^5$ V/cm.

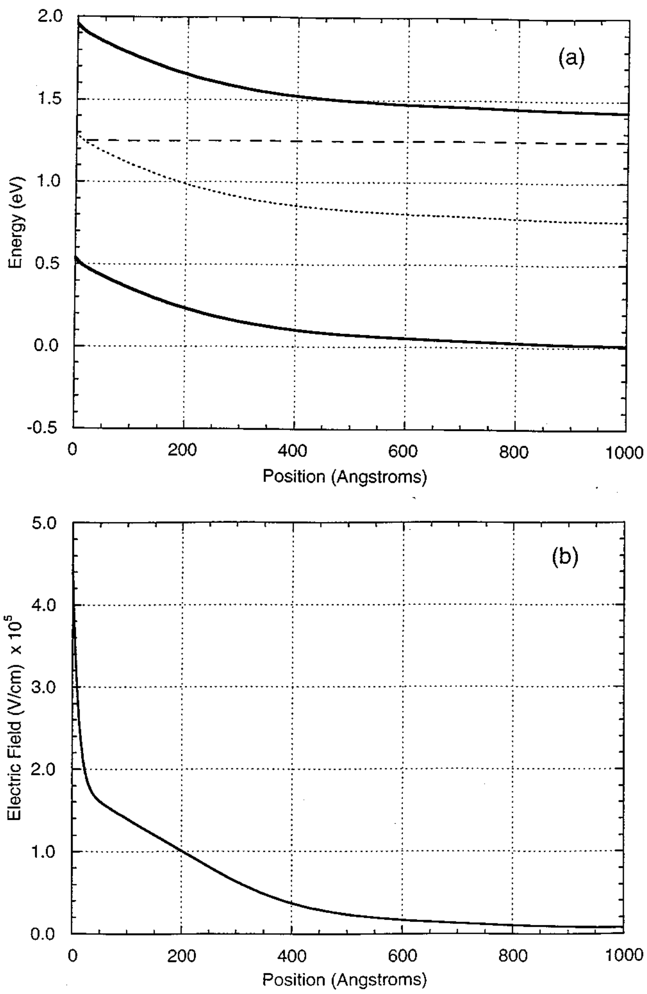

FIG. 3. Self-consistent Poisson's calculation of (a) the band profile and (b) the magnitude of the field distribution $E(z)$ as a function of position from the surface for LTG:GaAs for (a) a trap density (N_T) of 1×10^{20} cm^{-3} having a Gaussian distribution of states with width $\sigma(=0.2$ eV), the peak of the Gaussian distribution occurring 0.25 eV below the intrinsic Fermi level and (b) midgap surface Fermi level pinning.

We have numerically integrated Eq. (4b) with the computed $E(z)$ of Fig. 3(b) and find that $\mathrm{Re}\langle\Delta\epsilon\rangle\propto 0.4E_s$, which yields an effective electric field of 1.8×10^5 V/cm, in good agreement with our experimental result.

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(b)]. Thus, an ''effective depletion width'' can be evaluated if we assume that

$$E(z)=E_s e^{-\alpha_E z}, \tag{5}$$

where the quantity $1/\alpha_E$ can be considered as the effective depletion width. If Eqs. (4b) and (5) are used to yield $E=0.4E_s$, we find a value of $\alpha_E=22\times10^{-3}$ Å^{-1}, which corresponds to an effective depletion width of 45 Å. The above simple analytical function probably underestimates α_E. Therefore, we conclude that the effective depletion width $\leqslant$45 Å.

In conclusion, we have used RAS at 300 K to evaluate the sign and magnitude of the near surface field in LTG:GaAs (001). We also have performed a self-consistent Poisson's calculation to determine $E(z)$ and the energy band profile. In contrast to a conventional SCR, in our material the field $E(z)$ does not vary linearly with position. There is good agreement between our experimentally determined effective near surface electric field and the calculation (midgap surface Fermi level pinning), yielding an effective depletion width $\leqslant$45 Å. 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 surface Fermi level pinning effects in LTG:GaAs.

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