

**Burstein-Moss shift of  $n$ -doped  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InP}$** 

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We have evaluated the Burstein-Moss (BM) shift at 300 K in seven samples of  $n$ - $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  ( $1.3 \times 10^{16} \leq n \leq 3.9 \times 10^{19} \text{ cm}^{-3}$ ) lattice matched to InP using spectral ellipsometry in the range of 0.4–5.1 eV. The data have been fitted over the entire spectral range to a model reported by Holden *et al.* [in *Thermophotovoltaic Generation of Electricity*, edited by T. J. Coutts, J. P. Brenner, and C. S. Allman, AIP Conf. Proc. No. 460 (AIP, Woodbury, NY, 1999), p. 39], based on the electronic energy-band structure near critical points plus relevant discrete and continuum excitonic effects. A Fermi-level filling factor in the region of the fundamental gap has been used to account for the BM effect. While our data exhibit nonparabolic effects, with a blueshift of 415 meV for the most highly doped sample, we did not observe the Fermi-level saturation at 130 meV for  $n \geq 10^{19} \text{ cm}^{-3}$  reported by Tsukernik *et al.* [Proceedings of the 24th International Conference on the Physics of Semiconductors, *Jerusalem, 1998*, edited by D. Gershoni (World Scientific, Singapore, 1999)]. Our BM displacements are in agreement with a modified full-potential linearized augmented-plane-wave calculation [G. W. Charache *et al.*, *J. Appl. Phys.* **86**, 452 (1999)] plus possible band-gap-reduction effects.

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The study of the Burstein-Moss (BM) effect in  $n$ - $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  lattice matched to InP is important from both fundamental and applied points of view. Recently Tsukernik *et al.*<sup>1</sup> presented an investigation of the BM shift in this material based on thermionic emission and diffusion over a barrier and concluded that the BM change saturates at about 130 meV for  $n \geq 10^{19} \text{ cm}^{-3}$ . This observation was explained as a ‘‘Fermi-level saturation;’’ based on their results the authors called for a reexamination of existing theories. In contrast, Charache *et al.*<sup>2</sup> and Holden *et al.*<sup>3</sup> did not observe such a Fermi-level saturation in heavily doped  $n$ - $\text{In}_{0.66}\text{Ga}_{0.34}\text{As}$ . Structures based on highly  $n$ -doped  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  materials have been used for several kinds of semiconductor devices such as heterojunction bipolar transistors,<sup>4</sup> resonant-tunneling devices,<sup>5</sup> and Bragg reflectors for surface-emitting lasers.<sup>6</sup> For these kinds of applications it is highly desirable to have information about the position of the Fermi level relative to the conduction-band edge.

We present a study of the BM effect at 300 K in seven samples of  $n$ - $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  ( $1.3 \times 10^{16} \leq n \leq 3.9 \times 10^{19} \text{ cm}^{-3}$ ) lattice matched to InP using spectral ellipsometry. The data have been fitted using a comprehensive model<sup>3,7</sup> based on the electronic energy-band structure near critical points plus relevant discrete and continuum excitonic effects. The BM shift at the direct gap was accounted for using a Fermi-level filling factor in addition to the discrete and continuum excitonic terms.<sup>3</sup> The Fermi-level alteration exhibits

nonparabolic effects. However, in contrast to Ref. 1, we did not observe a Fermi-level saturation. Our results exhibit a blueshift of 415 meV for the highest doped sample ( $n = 3.9 \times 10^{19} \text{ cm}^{-3}$ ). The BM displacements of this work are in agreement with a modified full-potential linearized augmented-plane-wave (FLAPW) calculation<sup>2</sup> plus possible band-gap-reduction effects<sup>8,9</sup> and are consistent with the results of Holden *et al.*<sup>3</sup> in  $n$ - $\text{In}_{0.66}\text{Ga}_{0.34}\text{As}$ .

The seven  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  samples studied were grown on (001) InP substrates by a compact metal-organic molecular beam epitaxy system.<sup>10</sup> The lattice-matching parameter and composition were determined by x-ray measurements in a double-crystal diffractometer. The carrier concentrations were evaluated by Hall-effect measurements at room temperature to be  $1.3 \times 10^{16}$ ,  $2.3 \times 10^{17}$ ,  $5.0 \times 10^{18}$ ,  $5.8 \times 10^{18}$ ,  $2.0 \times 10^{19}$ ,  $2.3 \times 10^{19}$ , and  $3.9 \times 10^{19} \text{ cm}^{-3}$ . The first sample was unintentionally doped while the other samples were Sn doped.

The optical data in the range of 0.74–5.1 eV were taken using a JY-Horiba variable-angle phase-modulated ellipsometer. For the interval of 0.4–0.8 eV a variable-angle instrument, which used a Fourier-transform infrared reflectometer as a light source, was employed. Thus, there was some overlap between the two intervals. All the samples were measured with both 65° and 70° incidence angles. To remove the surface oxide an etching procedure was performed. Details are given in Ref. 7, except in this study the etch was a 1:1 mixture of HCl and methanol, followed by a quick rinse in methanol and a spray of deionized water.

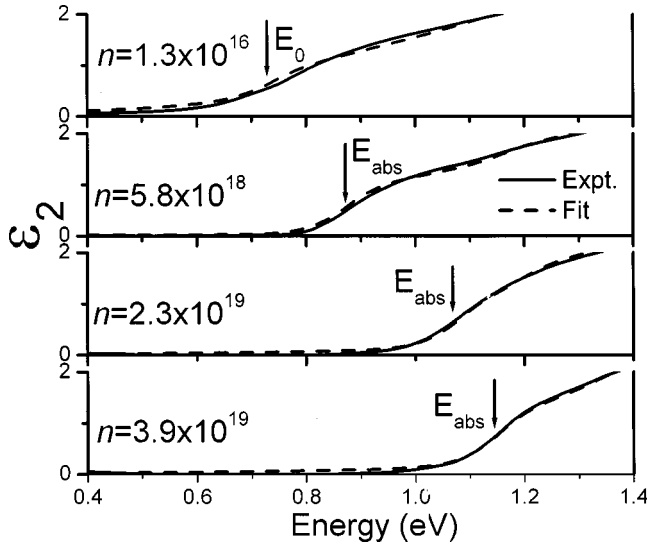


FIG. 1. The solid and dashed lines are the experimental and fitted values, respectively, of the imaginary part of the dielectric function  $\epsilon_2(E)$  in the region of the direct band gap for four of the samples studied. Indicated by arrows are the fundamental absorption edges obtained.

Even though our experiment was performed up to 5.1 eV, in this paper we deal only with the region near the fundamental band gap, leaving the interpretation of the higher-lying transitions for future work.

The solid lines in Fig. 1 are the experimental values of the imaginary part  $\epsilon_2$  of the dielectric function in the region of the direct gap ( $E_0$ ) corresponding to four of the samples. The data have been fitted using a comprehensive model based on the electronic energy-band structure near critical points plus relevant discrete and continuum excitonic effects.<sup>3,7</sup> In the fundamental absorption region the BM shift has been taken into account by the introduction of a Fermi-level filling factor (FLFF).<sup>3</sup> The quantity  $\epsilon_2$  in the region of the direct gap is thus written as<sup>3</sup>

$$\epsilon_2(E) = \frac{A}{\{1 + \exp[(E_{\text{abs}} - E)/kT]\}^2} \left[ \frac{R_0 \Gamma_0}{(E_0 - R_0 - E)^2 + \Gamma_0^2} + \int_{-\infty}^{\infty} \frac{\Theta(E' - E_0)}{1 - \exp[-2\pi z_1(E')]} \frac{\Gamma_0 dE'}{(E - E')^2 + \Gamma_0^2} \right], \quad (1)$$

where  $E$  is the photon energy, the term  $\{1 + \exp[(E_{\text{abs}} - E)/kT]\}^{-1}$  is the FLFF,  $E_{\text{abs}}$  is the absorption edge,  $\Gamma_0$  is the broadening parameter for both the discrete and continuum exciton terms (these two parameters have been taken as equal),  $z_1(E) = [R_0/(E - E_0)]^{1/2}$ ,  $R_0$  is the exciton Rydberg energy,  $\Theta(E)$  is the unit step function, and “ $kT$ ” is explained below. In Eq. (1),  $A \propto (R_0)^{1/2} (\mu^*)^{3/2} |M_0|^2$ , where  $\mu^*$  is the reduced interband effective mass at  $E_0$  and  $M_0$  is the matrix element of the momentum between  $\Gamma_8^v$  and  $\Gamma_6^c$ . For  $\text{In}_{0.66}\text{Ga}_{0.34}\text{As}$   $R_0 = 3.5$  meV.<sup>3</sup> According to  $\mathbf{k} \cdot \mathbf{p}$  theory<sup>11</sup>  $R_0 \propto \mu^*$  and hence using the appropriate electron and heavy-hole masses from Ref. 12 we found  $R_0 = 4.0$  meV for our system. In Eq. (1) the first and second terms in the square brackets are the contributions of the discrete and continuum

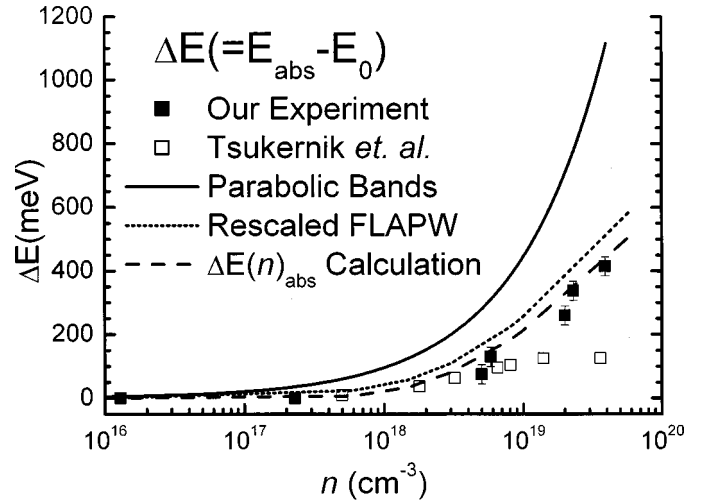


FIG. 2. The solid and open symbols are the BM shifts from our experiment and from Tsukernik *et al.* (Ref. 1), respectively. The solid and dotted lines are theoretical calculations of the BM shift according to parabolic-band theory and a rescaled FLAPW approach for  $\text{In}_{0.75}\text{Ga}_{0.25}\text{As}$ , respectively. The dashed line represents a calculation for  $\Delta E_{\text{abs}}(n)$  based on the rescaled FLAPW approach and the electron-electron interaction.

excitons, respectively. The values of  $\Gamma_0$  for the different samples increased monotonically with carrier concentration from 22 to 70 meV.

For the undoped sample the FLFF was not included so that for this case  $E_{\text{abs}} = E_0$ . In order to take into account inhomogeneous broadening, Eq. (1) with “ $kT$ ” set to its room-temperature value of 26 meV should be convoluted with a Gaussian. However, this is very difficult to do analytically, so to “simulate” inhomogeneous broadening we have used “ $kT$ ” as an adjustable parameter.<sup>3</sup> In Fig. 1, the dashed lines are the results of this fitting scheme and indicated by arrows are the absorption edge values  $E_{\text{abs}}$  obtained for each sample. This figure clearly displays the expected blueshift of  $E_{\text{abs}}$  with increasing carrier concentration. For the highest doped sample “ $kT$ ” = 35 meV. Using the room-temperature value of “ $kT$ ” = 26 meV results in a redshift of  $E_{\text{abs}}$  by only 6 meV, well within the experimental error. According to Ref. 3 the free-carrier absorption for  $n = 5.5 \times 10^{19} \text{ cm}^{-3}$  in this type of material starts to be considerable for energies below about 0.3 eV. We did not observe this effect and hence did not include it in our fitting procedure.

In Fig. 2 the solid and open squares are the experimental BM shifts of this experiment and those reported by Tsukernik *et al.*,<sup>1</sup> respectively. For our data, representative error bars are shown. Note that the BM shift of Ref. 1 saturates at about 130 meV. According to parabolic-band theory<sup>13,14</sup> the absorption edge shift  $\Delta E_{\text{abs}}$  is given by

$$\Delta E_{\text{abs}} = E_{\text{abs}} - E_0 = \left( \frac{\hbar^2}{2\mu^*} \right) [3\pi^2 n]^{2/3} - E_{\text{BGR}}, \quad (2)$$

where  $E_{\text{BGR}}$  is due to the band-gap-reduction effect. Using Eq. (2) with conduction and heavy-hole effective masses of

0.0432 and 0.303 (in units of the free-electron mass), respectively,<sup>12</sup> and neglecting  $E_{\text{BGR}}$ , we have obtained the solid curve in Fig. 2.

Charache *et al.*<sup>2</sup> have reported a FLAPW determination of the BM shift, including nonparabolic effects, in  $n\text{-In}_{0.75}\text{Ga}_{0.25}\text{As}$ . However, for  $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$  there is no such calculation. Thus, in order to get an approximation for this influence we have modified the FLAPW calculation for  $n\text{-In}_{0.75}\text{Ga}_{0.25}\text{As}$  of Ref. 2 by the factor  $\mu_{0.75}^*/\mu_{0.53}^*$ . For  $\text{In}_{0.75}\text{Ga}_{0.25}\text{As}$  we used conduction and heavy-hole masses of 0.0335 and 0.288,<sup>12</sup> respectively (in units of the free-electron mass). This rescaled FLAPW calculation is shown by the dotted line in Fig. 2.

In order to evaluate the band-gap reduction due to electron-electron interaction ( $\Delta E^{e-e}$ ) we have used<sup>15</sup>  $\Delta E^{e-e} \sim n^{1/3}/\epsilon_r(0)$ , where  $\epsilon_r(0)$  is the real part of the static dielectric constant. Considering that<sup>15</sup>  $\Delta E^{e-e}(\text{InP}) = 2.25 \times 10^{-8} n^{1/3}$  eV,  $\epsilon_r(\text{In}_{0.53}\text{Ga}_{0.47}\text{As}) \approx 13.9$ ,<sup>16</sup> and  $\epsilon_r(\text{InP}) \approx 12.56$ ,<sup>16</sup> it follows that  $\Delta E^{e-e}(\text{In}_{0.53}\text{Ga}_{0.47}\text{As}) = 2.03 \times 10^{-8} n^{1/3}$  eV.

Subtracting  $\Delta E^{e-e}(\text{In}_{0.53}\text{Ga}_{0.47}\text{As})$  from the FLAPW calculation, we obtain the dashed line shown in Fig. 2, which provides a description for  $\Delta E_{\text{abs}}(n)$  as a function of the carrier concentration. The small differences between the calculation for  $\Delta E_{\text{abs}}(n)$  and our experimental data in Fig. 2 are probably due to other band-gap-reduction effects not considered, such as band tailing.

The band-gap narrowing for concentrations of  $n \sim 3.5 \times 10^{19} \text{ cm}^{-3}$  is estimated to be around 100 meV for GaAs (Ref. 8) and InAs.<sup>9</sup> We therefore assume that the band-gap-narrowing effect for this carrier concentration in our case should also be  $\sim 100$  meV. Subtracting  $E_{\text{BGR}} = 100$  meV from the rescaled FLAPW calculation, we obtain that the

expected shift should be about 314 and 413 meV for  $n = 2.3 \times 10^{19}$  and  $n = 3.9 \times 10^{19} \text{ cm}^{-3}$ , respectively. Comparing these values with the experimental ones, i.e., 338 and 415 meV, respectively, a good agreement is obtained. From Fig. 3 of Ref. 6 the Fermi-level shifts for  $n \sim 4 \times 10^{18}$  and  $7 \times 10^{18} \text{ cm}^{-3}$  are 55 and 125 meV, respectively. These values are in good agreement with our values of 75 and 130 meV obtained for  $n = 5.0 \times 10^{18}$  and  $5.8 \times 10^{18} \text{ cm}^{-3}$ , respectively.

From Fig. 2 it follows that the BM shift in this system exhibits nonparabolic effects. However, contrary to Ref. 1, we have not observed any saturation of the Fermi level. The disagreement between our results and those of Tsukernik *et al.* can probably be attributed to the complexity and approximations used in their analysis of the thermionic emission and diffusion technique. On the other hand, the interpretation of the ellipsometric data is relatively straightforward.

In conclusion, we have evaluated the BM effect at 300 K in seven samples of  $n\text{-In}_{0.53}\text{Ga}_{0.47}\text{As}$  ( $1.3 \times 10^{16} \leq n \leq 3.9 \times 10^{19} \text{ cm}^{-3}$ ) lattice matched to InP using spectral ellipsometry. The Fermi-level shift exhibits nonparabolic effects. However, in contrast to Ref. 1, we did not observe a Fermi-level saturation. Our results exhibit a blueshift of 415 meV for the most highly doped sample ( $n = 3.9 \times 10^{19} \text{ cm}^{-3}$ ). The BM displacements of this work are in agreement with a calculation based on a modified FLAPW approach plus possible band-gap-reduction effects and are consistent with the results of Holden *et al.* in  $n\text{-In}_{0.66}\text{Ga}_{0.34}\text{As}$ .

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