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## LETTER TO THE EDITOR

# Conduction-band universality in GaAs-based systems

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**Abstract.** The non-parabolicity of the conduction band is predicted by a Kane four-band calculation to be approximately universal in direct-gap GaAs under varying pressure, and in direct-gap $Al_xGa_{1-x}As$ for various compositions $x$, when the band dispersion is plotted in natural units of effective Rydbergs and effective lattice constants. The predicted universality is expected to be a better approximation than the Kane approximation itself.

It has recently been pointed out [1] that the conduction band structure of the common III–V semiconductor compounds exhibits a non-parabolicity which is universal, to a good approximation, when the dispersion is plotted in the natural units of effective Rydbergs Ry* and effective Bohr radii $a^*$, where

$$\mathrm{Ry}^* = e^2/2\epsilon a^* \tag{1}$$

and

$$a^* = \hbar^2\epsilon/m^* e^2 . \tag{2}$$

Here $m^*$ is the $k = 0$ conduction-band effective mass, $k$ the wavenumber, $e$ the magnitude of the electronic charge, and $\epsilon$ the static dielectric constant.

It is natural to expect that a property which appears to be common among the III–V semiconductors will also hold for closely related systems. It will be shown here that there is good reason for expecting this to be the case for GaAs under pressure and for $Al_xGa_{1-x}As$ as a function of composition.

The conduction band of a direct-gap semiconductor near the Γ-point will be approximated here by the three-level (four-band) Kane [2] approximation

$$E'(E' + E_G)(E' + E_G + E_{SSO}) - k^2P^2\,(E' + E_G + \tfrac{2}{3}E_{SSO}) = 0 \tag{3}$$

where the electron energy $E$ is given by

$$E = E' + \frac{\hbar^2k^2}{2m_e} . \tag{4}$$

Here $E_G$ is the energy of the valence-band maximum and $E_{SSO}$ the maximum of the spin-split-off band, referred to an energy zero at the bottom of the conduction band. This approximation has the advantage that changes in band structure due to variations in pressure or composition can be incorporated simply; the effectiveness of the approximation itself is addressed hereafter.

The Kane [2] momentum matrix element $P$ can be obtained from experiment. It can also be estimated to good accuracy by fitting it to the $k = 0$ effective mass: explicitly,

$$P = \frac{\hbar^2}{2m^*}\,\frac{E_G(E_G + E_{SSO})}{E_G + 2E_{SSO}/3}\left(1 - \frac{m^*}{m_e}\right) . \tag{5}$$

The latter procedure was chosen here, and the relevant band structures calculated using as input experimental values for $E_G$, $E_{SSO}$, $m^*$, $\epsilon$ and lattice constant $a$, together with the experimental dependence of these quantities upon hydrostatic pressure $p$ in pure GaAs, or upon composition $x$ in $Al_xGa_{1-x}As$.

For pure GaAs, the pressure dependence of $E_G$ and $E_{SSO}$ has been taken from Shantharama *et al* [3], and that of $m^*$ from O'Reilly *et al* [4]. The pressure dependence of the static dielectric constant was taken to be [5] $\epsilon(p) = \epsilon(0) - 1.73 \times 10^{-3}p$, with pressure $p$ in kbar. The composition dependence of $E_G$ for $Al_xGa_{1-x}As$ has been taken from Peakes *et al* [6], and that for $E_{SSO}$, $m^*$ and $\epsilon$ from Adachi [7].

The composition dependence of the conduction band of $Al_xGa_{1-x}As$ calculated from equations (3)–(5)

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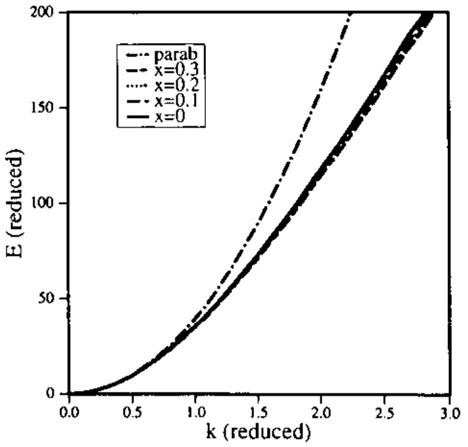

**Figure 1.** Conduction band dispersion in direct-gap $Al_xGa_{1-x}As$ for four aluminium compositions $x$, plotted in reduced units, from equations (2) and (3): $E$ in units of Ry* and $k$ in units $(2\pi/a^*)$. The common parabolic prediction is also shown (chain curve).

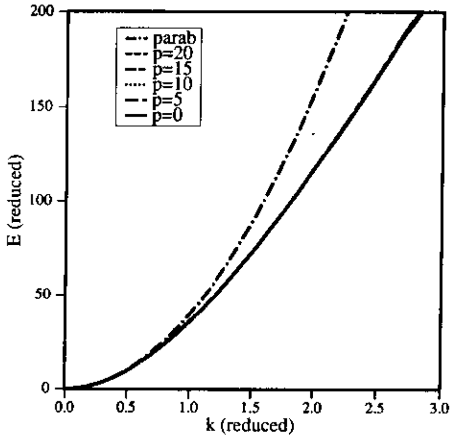

**Figure 2.** Conduction band dispersion in pure GaAs under hydrostatic pressure $p$ (five equal steps from 0 to 20 kbar) in the reduced units of figure 1, from equations (2) and (3); the curves appear indistinguishable. The chain curve is again the parabolic prediction.

is shown in figure 1 for four different Al concentrations $x$ from $x = 0$ to $x = 0.3$ (covering most of the composition range for which AlGaAs is a direct-gap material). Dispersion is plotted in natural units (equations (1) and (2)), for $k$ values up to about 0.1 of a Brillouin zone. Deviation from parabolicity is considerable, but the calculated AlGaAs band structures are virtually indistinguishable from each other in these units.

Figure 2 shows similar plots for GaAs under various degrees of hydrostatic pressure from 0 to 20 kbar. Non-parabolicity of these band structures is predicted to be universal to an even better approximation than in figure 1: all five curves agree to near-graphical accuracy.

Some feeling for the extent to which universality plays a part in what are in any case rather similar band structures may be gained from figure 3. Here the dispersion following from equations (3) and (4) is plotted in 'real' units (meV and $\text{Å}^{-1}$) for the highest pressure (20 kbar), and the maximum Al concentration ($x = 0.3$), considered (parabolic $E$–$k$ curves are not plotted, since

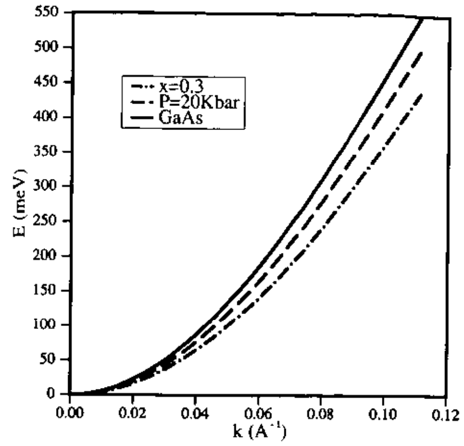

**Figure 3.** Conduction band dispersion from equations (2) and (3) in units of meV and $\text{Å}^{-1}$, for pure GaAs (solid curve) and $Al_{0.3}Ga_{0.7}As$ (chain curve) at ambient pressure, and GaAs at a pressure of 20 kbar (broken curve). Lines cover approximately 0.1 of the Brillouin zone.

they should be different for each of the three cases given, in these units). Figure 3 shows the same $E$–$k$ range as figures 1 and 2. Thus differences of band structure which are significant when given in terms of standard dimensional units virtually disappear when the natural units of equations (1) and (2) are used.

The exceptional degree of uniformity in band structure of GaAs under hydrostatic pressure can be related to the fact that both the Kane [2] momentum matrix element $P$ and the static dielectric constant are approximately unchanged under application of hydrostatic pressure. It has been shown in [1] that the Kane cubic band structure of equation (3) is well approximated by a two-band model,

$$E'(E' + E_{\text{eff}}) - k^2P^2 = 0 \tag{6}$$

where

$$E_{\text{eff}} = E_{\text{G}}(E_{\text{G}} + E_{\text{SSO}})/(E_{\text{G}} + \tfrac{2}{3}E_{\text{SSO}}) \,. \tag{7}$$

As pointed out in [1], when the free-electron correction is neglected, equation (6) is rigorously universal in the scaled variables $E/P^2m^*$ and $k/Pm^*$, and would also be rigorously universal in the natural units of equations (1) and (2) if the product $P\epsilon$ were constant. Since this product changes by less than 1% in GaAs for pressure changes of up to 20 kbar, it is hardly surprising that the high-pressure band structure of GaAs should behave universally in reduced variables to a high degree of accuracy.

Finally it is necessary to consider the limits imposed on the present conclusions by the use of the Kane [2] approximation. One might expect the approximation itself to be good for $k$ values no greater than a tenth of a Brillouin zone. At 0.1 of a zone the Kane approximation (2), (3) for GaAs still agrees with a detailed experimental pseudopotential calculation [1], using an 89 plane-wave basis, to within 20 meV in about 500, along the [100] direction. The approximation is less satisfactory along [111], however, and agreement to within 5% with the pseudopotential calculation only holds within 5% of the zone.

There is nevertheless good reason to expect that that universality itself will be evident in the [111] direction for the compounds considered here. Figure 1 of [1] shows an agreement among the relevant [111] conduction band structures that is good to about 0.7% for GaAs at 0.1 of a zone (note that InP is beyond a tenth of its zone at this reduced wavevector and must be excluded from the comparison). In other words, the predicted universality [1] for the relevant III–V's is an order of magnitude better approximation than the Kane approximation itself, for GaAs at a tenth of a zone. A better calculation of the GaAs-based band structures considered above is thus of great interest, but should also be expected to show the universality predicted here.

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