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LETTER TO THE EDITOR

An EPM calculation of band structure of zincblende semiconductor alloys

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Abstract. The band structures of several zincblende semiconductor alloys are calculated in the virtual crystal approximation using the empirical pseudopotential method (EPM). We propose an interpolation scheme for the pseudopotential form factors that applies universally well to various zincblende semiconductor alloys. The calculated results are in good agreement with experiments, where the lattice mismatch is large. For the case of small lattice mismatch, it appears necessary to include the disorder effect.

The electronic band structure of ternary compound semiconductors is of considerable theoretical and experimental interest. Although more recent and more refined methods like the coherent potential approximation (Gupta *et al* 1987) and the all-electron mixed-basis approach (Bernard and Zunger 1987) may produce more accurate values of the band structure, the empirical pseudopotential method (EPM) within the virtual crystal approximation (VCA) still offers the simplest, yet reasonably accurate, means of obtaining the overall band structure of alloys.

Although EPM calculations are generally proven to produce reasonably good band structures, the results of various calculations are not in universal agreement. Richardson (1971) reported general overbowing, whereas others obtained underbowing of the energy gaps (Baldereschi *et al* 1977, Schulze *et al* 1976). Generally, this discrepancy is attributed to the disorder effect. However, we show that this type of discrepancy can also arise from the interpolation process of the form factors that becomes necessary because of the lattice mismatch. Therefore, it is essential to provide a correct interpolation scheme before the disorder effect is included in the calculation. In this Letter, we address this problem.

The present method for the calculation of the band structure of the alloy semiconductors, A_xB_{1-x} , is based on the model proposed by Richardson (1971).

The EPM form factors for the alloy A_xB_{1-x} within the VCA is written

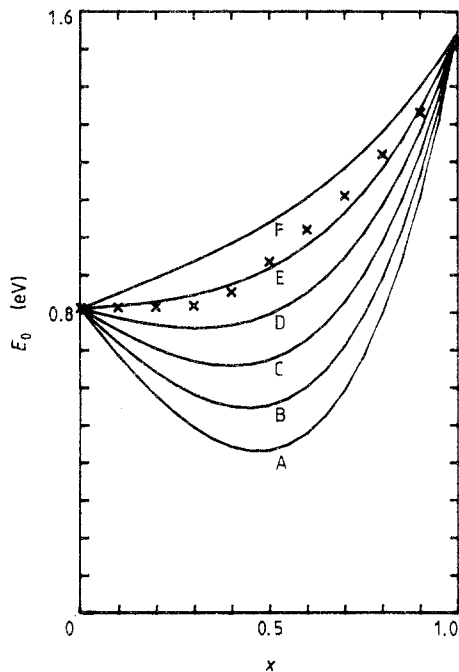
$$V_{\text{alloy}} = (1/\Omega_{\text{alloy}})[x\Omega_A V_A(G) + (1-x)\Omega_B V_B(G)]. \quad (1)$$

The terms $V_A(G)$ and $V_B(G)$ cannot be taken directly from Cohen and Bergstresser (1966), since corrections must be made for the change in G -values due to the change in the lattice constant. Richardson fitted the pure compound form factors to simple cubics

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Table 1. Pseudopotential form factors (in Ryd) and lattice constants (in Å) used in the calculation, after Cohen and Bergstresser (1966) (see text).

	GaAs	GaSb	InAs	GaP	InSb	AlAs
V_3^s	-0.235	-0.220	-0.220	-0.224	-0.200	-0.230
V_8^s	0.011	0.002	0.049	0.033	0.0	0.026
V_{11}^s	0.062	0.050	0.049	0.072	0.043	0.071
V_3^A	0.071	0.060	0.079	0.120	0.034	0.105
V_4^A	0.050	0.050	0.047	0.070	0.024	0.065
V_{11}^A	0.010	0.010	0.029	0.020	0.010	0.005
a	5.653	6.095	6.058	5.450	6.478	5.661

**Figure 1.** Calculated values of the energy gap E_0 of $\text{GaSb}_{1-x}\text{As}_x$ are shown for various values of V_{12} ($V_{12} = pV_{11}$): Curve A, $p = 0$; curve B, $p = 0.2$; curve C, $p = 0.4$; curve D, $p = 0.6$; curve E, $p = 0.8$; curve F, $p = 1.0$. \times , experimental values from Takeshima (1979).

from which V_A and V_B corresponding to the new G values are calculated. His calculation generally produced overbending of the energy gaps. This simple procedure does not work well when the lattice mismatch is substantial, because we need form factors for G^2 smaller than 3 and larger than 11. A form factor for G^2 smaller than 3 is not sensitive to the small change of G . However form factor for G^2 larger than 11 is quite sensitive to the variation of G , because it has a maximum near $G^2 = 11$ (Cohen and Heine 1970). This indicates that a careful interpolation scheme is required near $G^2 = 11$.

In the usual EPM calculation, form factors for G^2 equal to and larger than 12 are set zero. However, this does not mean V_{12} goes to zero literally. Rather, this approximation is taken in the spirit of truncation or 'folding down' of a large matrix (Cohen and Heine 1970). Therefore, it is necessary to use a non-zero value of V_{12} in the interpolation scheme for the form factors near $G^2 = 11$, while it is still necessary to set V_{12} equal to

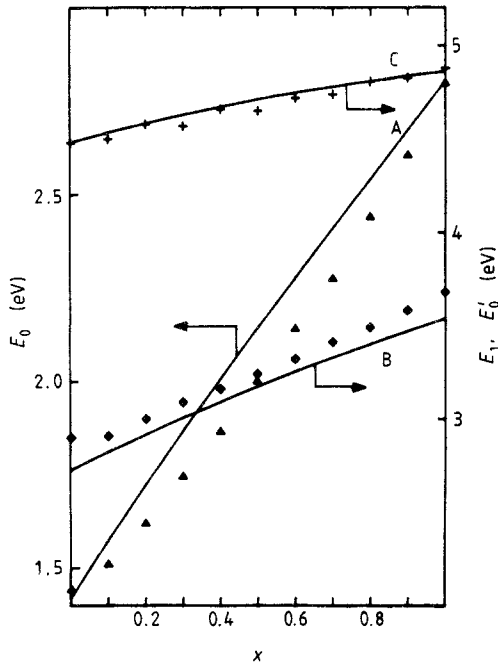


Figure 2. Calculated values of energy gaps E_0 (curve A), E_1 (curve B), and E'_0 (curve C) of $\text{GaAs}_{1-x}\text{P}_x$ compared with experiments. Experimental values are taken from Vishnubhatia *et al* (1969).

zero for the band calculation of alloys. To see the effect of V_{12} variation on the energy gaps, we calculated the band structure of $\text{GaSb}_{1-x}\text{As}_x$ varying V_{12} from zero to $V_{12} = V_{11}$ systematically.

Pseudopotential form factors for the pure compounds listed in table 1 are taken from Cohen and Bergstresser (1966), but slightly modified to fit more recent experimental data. For the interpolation of the form factor of $\text{GaSb}_{1-x}\text{As}_x$, we write $V_{12} = pV_{11}$ and vary p from 0 to 1 using an interval of 0.2. In figure 1, we show the result of the calculation. The result clearly demonstrates that zero is not a proper choice for V_{12} in the interpolation. Here, it is shown that a calculation based on $V_{12} = 0.8 V_{11}$ produces the best agreement with experimental results. We have carried out the band-gap calculations on various alloys using the relation $V_{12} = 0.8 V_{11}$. From figures 2 and 3, we observe that the calculated results for various direct and indirect gaps are generally in good agreement with experiments. Exceptions to this rule are $\text{Ga}_{1-x}\text{Al}_x\text{As}$ and also, to a lesser degree, $\text{GaAs}_{1-x}\text{P}_x$. The linear behaviour of the E_0 gap of $\text{Ga}_{1-x}\text{Al}_x\text{As}$ is found not to change significantly when p is changed from 0 to 1.

It may appear contradictory that these alloys, which have smaller lattice mismatches and, thus, smaller uncertainties in the interpolation, should have larger discrepancies between theory and experiment. However, it can be easily understood if we consider the local atomic arrangement of the alloys. In the case of alloys with a large size mismatch, the tendency to order is strong, whereas with a smaller mismatch, disorder becomes much greater. Therefore, it appears necessary to include the effect of disorder if one is to obtain agreement between theory and experiment for $\text{Ga}_{1-x}\text{Al}_x\text{As}$ and $\text{GaAs}_{1-x}\text{P}_x$. Indeed, Bernard and Zunger (1987) found that the disorder contribution to the bowing parameter is small for the alloys with a large size mismatch.

In conclusion, we have presented an EPM calculation of the energy band gaps of zincblende semiconductor alloys. It is shown that the bowing of the band gaps is well

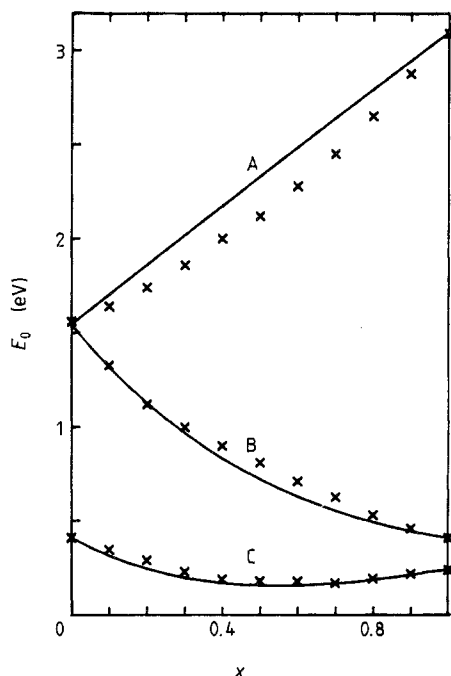


Figure 3. Calculated values of E_0 gaps of three semiconductor alloys (full curves) compared with experiments (\times). Curve A, $\text{Ga}_{1-x}\text{Al}_x\text{As}$; curve B, $\text{Ga}_{1-x}\text{In}_x\text{As}$; curve C, $\text{InAs}_{1-x}\text{Sb}_x$. Experimental values for $\text{Ga}_{1-x}\text{In}_x\text{As}$ and $\text{InAs}_{1-x}\text{Sb}_x$ are taken from Van Vechten *et al* (1972) and for $\text{Ga}_{1-x}\text{Al}_x\text{As}$ from Dingle *et al* (1987).

represented by assuming $V_{12} = 0.8 V_{11}$ in the interpolation scheme. Exceptions arise when the lattice mismatch is small. In such cases, the effect of disorder is expected to be large and should be considered separately. The work on this problem within the EPM is in progress and will be reported elsewhere.

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