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Band structure of ternary compound semiconductors beyond the virtual crystal approximation

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Abstract. A simple pseudopotential scheme, which incorporates compositional disorder as an effective potential, is proposed for calculation of the band structure of ternary compound semiconductors. It is shown that the present theory, which is free from any additional parameter, satisfactorily produces the band-gap bowings of ternary compounds when the lattice mismatch is small.

1. Introduction

The electronic band structure of ternary compound semiconductors is of considerable theoretical and experimental interest. Although several elaborate approaches (Wei and Zunger 1989, Krishnamurthy *et al* 1988) may produce better values for the band structures, still the empirical pseudopotential method (EPM) within the virtual crystal approximation (VCA) offers the simplest, and yet a reasonably accurate, means of obtaining the overall band structure of the alloys. However, at the same time, the VCA is known to lead to bowing parameters of the main gap that are too weak to account for experimental results. To remedy this shortcoming, it is necessary to include the disorder effect in the VCA. Baldereschi and Maschke (1975) treated the compositional disorder effect as a perturbation and calculated up to the second order within the VCA approach. However, this perturbative approach was not completely satisfactory in explaining the band-gap bowings (Baldereschi *et al* 1977). Also, the computational efforts required for this method is substantial, thus making the application of this method rather difficult. In this paper we propose a simple pseudopotential scheme which includes the compositional disorder into the VCA approach. Our scheme employs the local EPM and includes the disorder effect by introducing an effective disorder potential. Since, the present method is non-perturbative, it is as simple as the original EPM calculation.

2. Effective disorder potential

We consider a mixed crystal $A_xB_{1-x}C$. Here, we assume that all C atoms occupy the proper positions. Thus, in the following, we treat the crystal made of AC molecules of fraction x and BC molecules of fraction $1 - x$. The potential of the alloy is given by

$$V(\mathbf{r}) = V_{vc}(\mathbf{r}) + V_{dis}(\mathbf{r}) \quad (1)$$

where V_{vc} is the periodic virtual crystal potential and V_{dis} is the non-periodic potential

due to the compositional disorder. V_{dis} for a particular distribution is given by (Baldereschi and Maschke 1975)

$$V_{\text{dis}}(\mathbf{r}) = (1-x) \sum_{j_A} \Delta(\mathbf{r} - \mathbf{R}_j) - x \sum_{j_B} \Delta(\mathbf{r} - \mathbf{R}_j) \quad (2)$$

where $\Delta(\mathbf{r}) = V_{\text{AC}}(\mathbf{r}) - V_{\text{BC}}(\mathbf{r})$. Here j_A indicates that the summation on j is carried out on the AC molecular sites only, and j_B on BC molecular sites only.

The conventional VCA makes the following approximations

$$\sum_{j_A} \Delta(\mathbf{r} - \mathbf{R}_j) = x \sum_j \Delta(\mathbf{r} - \mathbf{R}_j) \quad \sum_{j_B} \Delta(\mathbf{r} - \mathbf{R}_j) = (1-x) \sum_j \Delta(\mathbf{r} - \mathbf{R}_j).$$

This approximation makes V_{dis} disappear and $V(\mathbf{r})$ becomes equal to $V_{\text{VC}}(\mathbf{r})$. Instead, here, we introduce the disorder effect by assuming that $\sum_{j_A} \Delta(\mathbf{r} - \mathbf{R}_j) = \alpha x \sum_j \Delta(\mathbf{r} - \mathbf{R}_j)$ and $\sum_{j_B} \Delta(\mathbf{r} - \mathbf{R}_j) = \beta(1-x) \sum_j \Delta(\mathbf{r} - \mathbf{R}_j)$, where α and β are disorder functions dependent on the concentration x and the potential energy. The concentration dependence of α and β is easy to understand. For example, α will be equal to unity when $x = 1$. However, when $x \neq 1$, α should be other than unity, so that it does not become identical with VCA.

With this approximation, the disorder potential is given by

$$V_{\text{dis}}(\mathbf{r}) = (\alpha - \beta)x(1-x) \sum_j \Delta(\mathbf{r} - \mathbf{R}_j). \quad (3)$$

This approximation is analogous to the single-site approximation of the self-energies in the CPA approach and replaces the random fluctuating potential by a periodic effective disorder potential (Chen and Sher 1981). A simple way of utilising equation (3) is to neglect the concentration dependence of $\alpha - \beta$ and to treat it as an adjustable parameter. This type of approximation coupled with an empirical tight-binding method was tried by Porod and Ferry (1983). Although their method was successful in describing the band-gap bowings of ternary and quaternary semiconductor alloys, it is not supported by any physical justification in neglecting the concentration dependence.

In this paper, we show that the concentration dependence of $\alpha - \beta$ can be evaluated by considering an ensemble average of the potential energy deviation from the VCA value. For this purpose, we first assume that, except for the nearest-neighbour (NN) sites from the origin, all lattice sites are occupied by the virtual molecules which have the potential energy of V_{VC} . For the NN sites, we assume that the sites can be occupied by any particular combination of AC and BC molecules. With this assumption, we now evaluate the root mean square deviation of the potential energy from the VCA value (Harrison 1966). First, it is obtained using the disorder functions α and β and, next, directly from the probability calculation.

$$\begin{aligned} \left\langle \left(\sum_{j_A} \Delta(\mathbf{r} - \mathbf{R}_j) - x \sum_j \Delta(\mathbf{r} - \mathbf{R}_j) \right)^2 \right\rangle^{1/2} &= |(\alpha - 1)xN\Delta(d)| \\ &= \left(\sum_{n=0}^N {}_N C_n x^n (1-x)^{N-n} (n - Nx)^2 [\Delta(d)]^2 \right)^{1/2}. \end{aligned} \quad (4)$$

Here d is the NN distance and N the number of NN sites. Similarly, we obtain

$$|(\beta - 1)(1-x)N\Delta(d)| = \left(\sum_{n=0}^N {}_N C_n (1-x)^n x^{N-n} [n - N(1-x)]^2 [\Delta(d)]^2 \right)^{1/2}. \quad (5)$$

From these equations, we obtain the result

$$\alpha - \beta = \pm \frac{1}{N[x(1-x)]^{1/2}} \left(\frac{N^2(1-x)}{x} + \sum_{n=0}^N {}_N C_n x^{N-n-1} (1-x)^{n-1} [n^2 - 2nN(1-x)] \right)^{1/2}. \tag{6}$$

The second term in equation (6) can be simplified as follows:

$$\sum_{n=0}^N \binom{N}{n} x^{N-n-1} (1-x)^{n-1} [n^2 - 2nN(1-x)] = -N(N-1) + \frac{N^2(2x-1)}{x}. \tag{7}$$

Now equation (6) is simplified to

$$\alpha - \beta = \pm [x(1-x)N]^{-1/2}. \tag{8}$$

Here we assume that the disorder lowers the effective potential and, thus, we choose the negative sign for $\alpha - \beta$. The effective disorder potential is now given by

$$V_{\text{dis}}(\mathbf{r}) = - \left(\frac{x(1-x)}{N} \right)^{1/2} \sum_j \Delta(\mathbf{r} - \mathbf{R}_j). \tag{9}$$

Here N is 12 for the FCC structure. This result is not yet completely general, because we considered the compositional fluctuation from the NN site only. However, we shall find that the NN contribution is sufficient to account for the band-gap bowings satisfactorily. In fact, we can relax the above restriction by assuming that the next-NN sites are also occupied by a particular combination of real molecules and repeat a similar procedure as above to calculate $\alpha - \beta$. By repeating this procedure, we can include the whole crystal in the contribution. The final result is given by

$$V_{\text{dis}} = -P[x(1-x)]^{1/2} \sum_j \Delta(\mathbf{r} - \mathbf{R}_j) \tag{10}$$

where

$$P = \left(\frac{\sum_{i=1}^n N_i \Delta(d_i)^2}{\sum_{i=1}^n N_i \Delta(d_i)} \right)^{1/2}$$

Here i indicates the i th NNS and n can be extended to include the whole crystal. Although N_i becomes large and is approximately proportional to r^2 , the potential $\Delta(\mathbf{r})$ decreases more rapidly owing to screening, thus ensuring convergence of P . By adding this effective disorder potential to the virtual crystal potential, we have the final expression for the pseudopotential form factors:

$$V(G) = x(\Omega_{\text{AC}}/\Omega_{\text{alloy}})V_{\text{AC}}(G) + (1-x)(\Omega_{\text{BC}}/\Omega_{\text{alloy}})V_{\text{BC}}(G) - P[x(1-x)]^{1/2}(1/\Omega_{\text{alloy}})[\Omega_{\text{AC}}V_{\text{AC}}(G) - \Omega_{\text{BC}}V_{\text{BC}}(G)]. \tag{11}$$

3. Results and discussion

Since it is our aim to devise a simple and parameter-free theory to calculate the alloy band structure, we used equation (9) instead of equation (10). For numerical calculations, $V_{\text{AC}}(G)$ and $V_{\text{BC}}(G)$ should be corrected for the change in G -values due to the lattice constant variation (Lee *et al* 1989). Since our scheme does not include the lattice relaxation effect, we believe that it is most suitable for the materials with small lattice mismatches. Indeed, it is known that the compositional disorder effect is significant only when the lattice mismatch is small as in the cases of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ and $\text{GaAs}_{1-x}\text{P}_x$ (Bernard and Zunger 1987, Lee *et al* 1989).

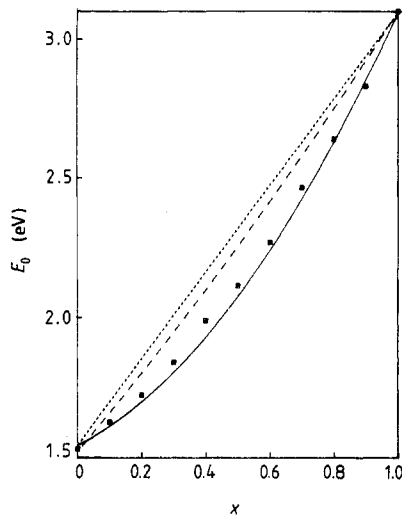


Figure 1. Calculated values of the E_0 gap for $\text{Al}_x\text{Ga}_{1-x}\text{As}$ are compared with experiments: ■, Dingle *et al* (1977); —, present theory; ····, without disorder; ---, experimental results of Bosio *et al* (1988) which can be fitted using equation (11) and $p = 0.11$.

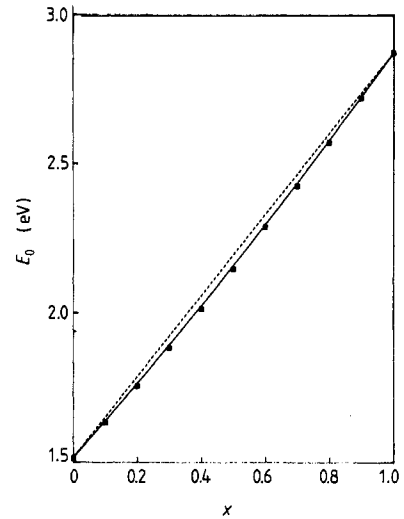


Figure 2. Calculated values of E_0 of $\text{GaAs}_{1-x}\text{P}_x$ are compared with experiment: ■, Nelson and Holonyak (1976); —, present theory; ---, without disorder.

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

	GaAs	GaP	AlAs
V_3^S (Ryd)	-0.235	-0.224	-0.230
V_8^S (Ryd)	0.011	0.033	0.026
V_{11}^S (Ryd)	0.062	0.072	0.071
V_3^A (Ryd)	0.071	0.120	0.105
V_4^A (Ryd)	0.050	0.070	0.065
V_{11}^A (Ryd)	0.010	0.020	0.005
a (Å)	5.653	5.450	5.661

In figures 1 and 2, we show the calculated band gaps of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ and $\text{GaAs}_{1-x}\text{P}_x$. The result shows clearly that, without the disorder potential, the EPM approach within the VCA does not produce the band-gap bowings. However, on adding the disorder potential (equation (9)) for $\text{Al}_x\text{Ga}_{1-x}\text{As}$ and $\text{GaAs}_{1-x}\text{P}_x$, excellent agreement with the experimental data has been obtained (Dingle *et al* 1977, Nelson and Holonyak 1976). In table 1, the form factors and lattice parameters used in the calculation are given. The form factors are taken from Cohen and Bergstresser (1966), but slightly modified to fit more experimental data (Lee *et al* 1989).

Recently Bosio *et al* (1988) reported an experimental result on $\text{Al}_x\text{Ga}_{1-x}\text{As}$, which has a much smaller bowing constant. Their result can be fitted satisfactorily by our theory if we use equation (11) and put $p = 0.11$. This indicates that the NN approximation may not be sufficient and, instead, we should use equation (11) and treat p as an adjustable parameter, if the results of Bosio *et al* are correct. However, since their result is confined

only to the direct gap of $\text{Al}_x\text{Ga}_{1-x}\text{As}$, it is not yet clear whether this small bowing constant represents the true experimental situation. Further experimental results on the direct and indirect gaps of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ and other ternary compound semiconductors appear necessary before we disregard the earlier data of Dingle *et al* (1977).

In conclusion, we have presented a simple pseudopotential scheme for the calculation of the band structure of ternary compound semiconductors. In this scheme, the compositional disorder is introduced as an effective disorder potential. This effective potential, which is parameter free, can be readily included in the conventional EPM calculation. It is shown that the bowings of the band gaps of $\text{Al}_x\text{Ga}_{1-x}\text{As}$ and $\text{GaAs}_{1-x}\text{P}_x$ can be produced satisfactorily using the present theory.

Acknowledgment

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