Effects of configurational, positional and vibrational degrees of freedom on an alloy phase diagram: a Monte Carlo study of $Ga_{1-x}In_xP$



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# Effects of configurational, positional and vibrational degrees of freedom on an alloy phase diagram: a Monte Carlo study of $Ga_{1-x}In_xP$

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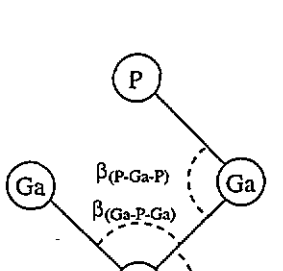
calculations [3] or from parametrized effective potentials [4, 5, 6, 8]. Both approaches are termed here as 'direct calculations'. In this paper we will consider insulating alloys (i.e. no

configurational and positional effects but, since only deterministic, energy-lowering atomic displacements are sought, dynamic vibrational effects are neglected. Thus it is analogous to CE-(b) in the context of cluster expansion.

Finally, in the third (D-(c)) level, one treats configurational and positional degrees of freedom on equal footing, e.g., by selecting random configurational changes ($\hat{S}$) and random

$$f_{Ga} = -0.4621$$
$$f_{In} = 0.9705. \quad (8)$$

Note that the various structures included in the fit correspond to a significant range ($\pm 0.3$Å) of atomic displacements, thus, in so far as the LDA is accurate, we can use our parametrized surface for calculating vibrations. In all our calculations, each atom is fourfold coordinated. The resulting $\beta$ values are given in the insert of figure 2. Since our VFF is fit also to




$\beta_{(P\text{-}In\text{-}P)}$ = 12.2975 N/m

$\beta_{(In\text{-}P\text{-}In)}$ = 0.1841 N/m

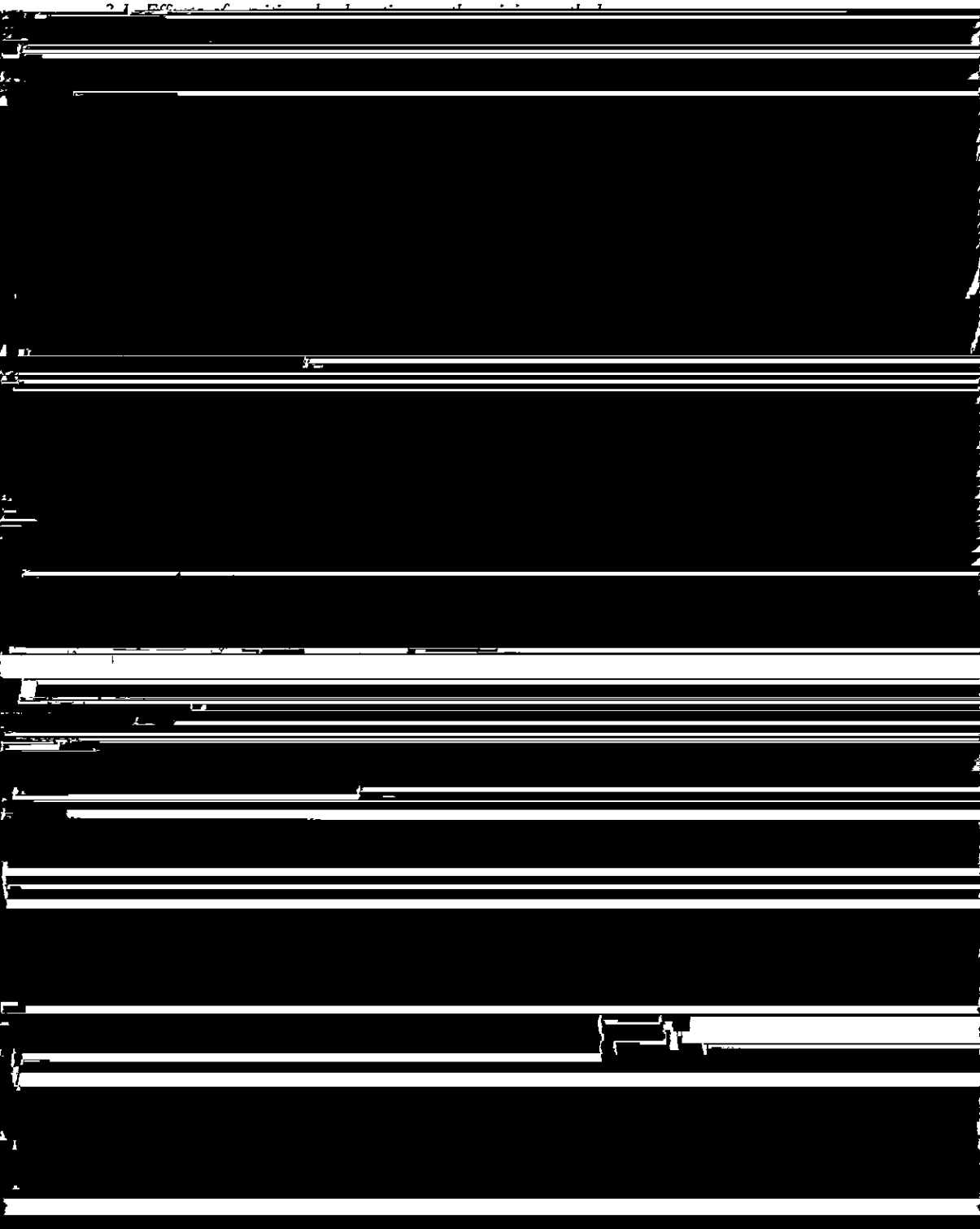
$\beta_{(Ga\text{-}P\text{-}In)}$ = 1.6715 N/m

chosen as the zinc-blende positions $\{R_i^0\}$ of a cubic cell with periodic boundary conditions and a Vegard lattice constant $a(x)$.

(ii) The displacement field is defined as follows: first, atoms (indexed by $i$) are chosen randomly. Subsequently, three types of Monte Carlo displacements/flips are introduced: (a) At each step, a random and small coordinate displacement $\Delta R_i$ is chosen, and the new positions $\{R_i'\}$ are mapped : $\{R_i'\} \rightarrow \{R_i\} + \Delta R_i$. (b) About every $1/P_S$ steps the spin $\hat{S}_i$ is flipped so $\{\hat{S}_i\}$ is mapped to $\{\hat{S}_i'\}$. (c) About every $1/P_V$ steps a random small volume change $\Delta V$ is chosen and the volume of the cell is mapped by $\{R_i'\} \rightarrow \{R_i\} + \{\Delta R_i\}$, where $\Delta R_i = (1, 1, 1)\Delta V$ for all $i$. Hence, $P_S$ and $P_V$ are the probabilities of spin flip and volume change respectively. We chose $P_S = 0.05$ and $P_V = 1/N$ where $N$ is the number

$8 \times N \times N \times N$ atoms for $5 \leqslant N \leqslant 8$, we estimate that finite-size errors are below 1% for both algorithms.

## 3. Results



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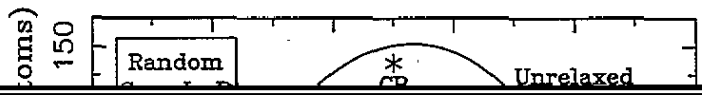
oms)
150
Random
Unrelaxed

tend to *lower* $T_{MG}$. The same trend was observed in empirical models that introduce vibrational effects into semiconductor alloy [36, 37] and noble metal alloy [38] phase diagrams. However, our *direct* calculation of vibrational effects suggests that previous

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[34] Glas F 1989 *J. Appl. Phys.* **66** 1667