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

1995 J. Phys.: Condens. Matter 7 1167

(http://iopscience.iop.org/0953-8984/7/6/018)

J. Phys.: Condens. Matter 7 (1995) 1167–1180. Printed in the UK

Effects of configurational, positional and vibrational degrees of freedom on alloy phase diagrams: a Monte

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

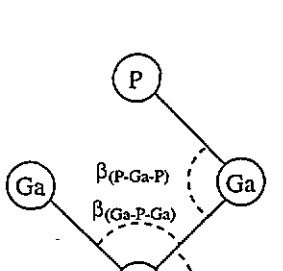
configurational and positional effects but, since only deterministic, energy-lowering atomic *displacements are sought, dynamic vibrational effects are neglected. Thus it is analogous* to CE-(b) in the context of cluster expansion.

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 $\{\hat{S}_i\}$ and *random* displacements $\{\Delta R_i\}$ during the statistical simulation. This D-(c) (direct, relaxed, dynamic) approach includes configurational, positional and vibrational effects.

Given a convenient Born–Oppenheimer surface E_{direct} one can either parametrize it in terms of a cluster expansion (equation (1)) and apply methods CE-(a) and CE-(b) or directly apply methods D-(a), D-(b) and D-(c), in conjunction with Monte Carlo simulations. The

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

Note that the various structures included in the fit correspond to a significant range (± 0.3Å) 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 β 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

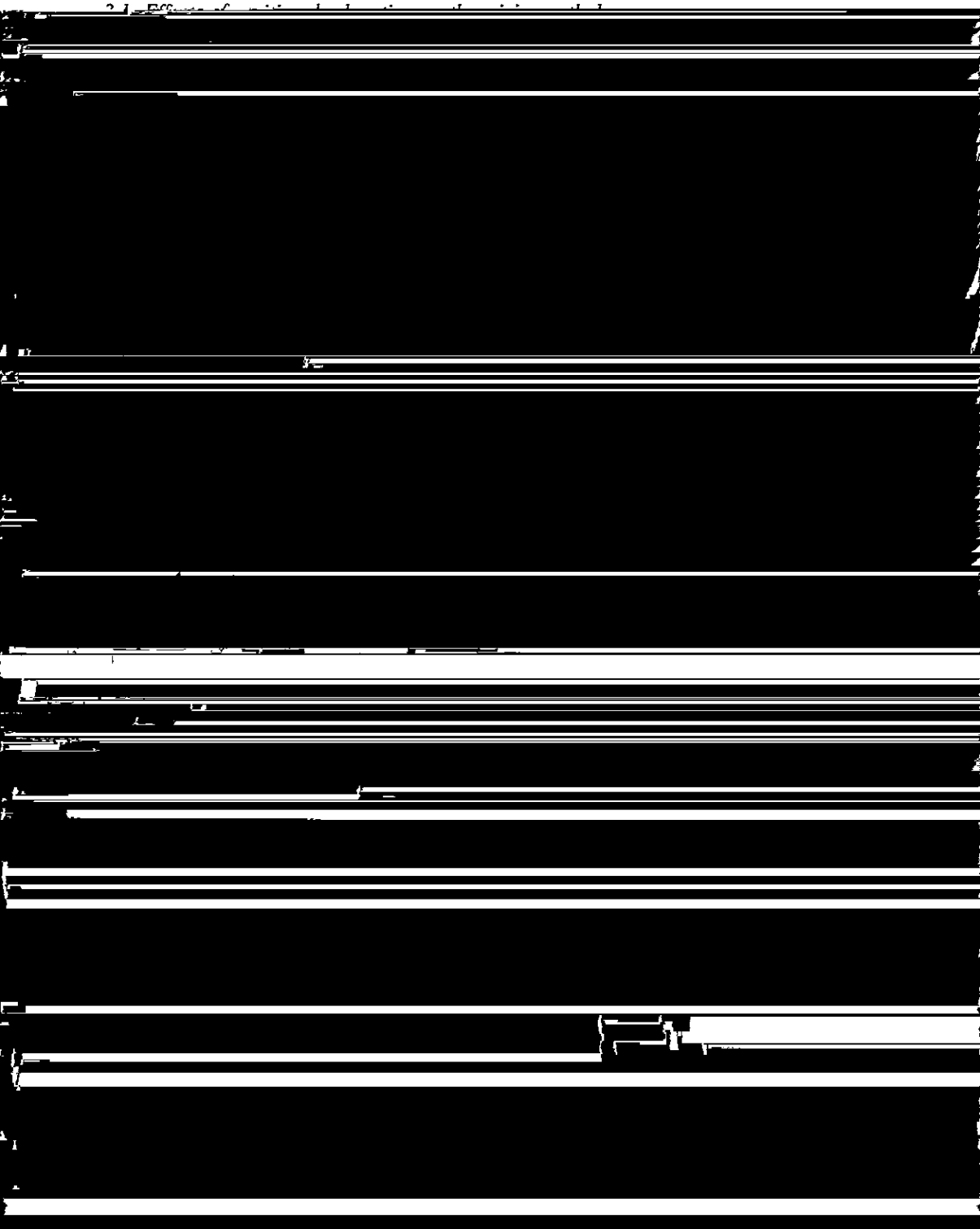
$\beta_{(Ga\text{-}P\text{-}In)}$ = 1.6715 N/m

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 ΔR_i is chosen, and the new

$8 \times N \times N \times N$ 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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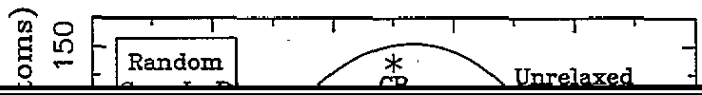
oms)
150
Random
Unrelaxed

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

supported by the US-Israel Binational Science Foundation under grant No. 88-00295. We

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