

Long-range order instead of phase separation in large lattice-mismatch isovalent A-B systems

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 (Received 1 October 2009; accepted 15 December 2009)

The formation of long-range order in large lattice-mismatch isovalent A-B systems is investigated using first-principles calculations. We find that the formation of long-range order is favored over phase separation in these systems. The formation of long-range order is observed in the case of the F-C₃F₂ system, where the lattice mismatch is 40%. The formation of long-range order is also observed in the case of the B₂O₃-B₂O (37%), B₂O₃-B₂O (30%), C₁-C₁ (20%), and B₂O₃-B₂O (33%) systems. The formation of long-range order is observed in ~60% of the cases.

DOI: 10.1103/PhysRevB.80.241202 PACS numbers: 61.50.Ah, 71.15

I. INTRODUCTION

In a homogeneous A_xB_{1-x}X system, the formation of long-range order is favored over phase separation. The formation of long-range order is observed in the case of the F-C₃F₂ system, where the lattice mismatch is 40%. The formation of long-range order is also observed in the case of the B₂O₃-B₂O (37%), B₂O₃-B₂O (30%), C₁-C₁ (20%), and B₂O₃-B₂O (33%) systems. The formation of long-range order is observed in ~60% of the cases.

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II. STRAIN RELEASE THROUGH COORDINATION NUMBER DISPROPORTIONATION

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$$\Delta H = \Delta E_D + \Delta E_{\text{dis}} + \Delta E_{\text{LP}} \quad (1)$$

$\Delta E_D = [x E_{AX}(\bar{V}) + (1-x) E_{BX}(\bar{V})]$
 $\bullet [x E_{AX}(V_{AX}) + (1-x) E_{BX}(V_{BX})]$

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