

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

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 (Received 11 October 2009; accepted 15 December 2009)

Abstract: We study the phase behavior of isovalent A_xB_{1-x}X systems with large lattice mismatch. The phase diagram shows a region of long-range order (LRO) instead of phase separation. The LRO region is bounded by a critical composition of approximately 40% A (x ≈ 0.4). The phase diagram also shows regions of phase separation (B_x-B (30%), C₁-C₁ (20%), and C₁-C₂ (33%)) and a region of long-range order (LRO) (~60%).

DOI: 10.1103/PhysRevB.80.241202 PACS: 61.50.Ah, 71.10.Fd

I. INTRODUCTION

We study homogeneous A_xB_{1-x}X systems with large lattice mismatch. The phase diagram shows a region of long-range order (LRO) instead of phase separation. The LRO region is bounded by a critical composition of approximately 40% A (x ≈ 0.4). The phase diagram also shows regions of phase separation (B_x-B (30%), C₁-C₁ (20%), and C₁-C₂ (33%)) and a region of long-range order (LRO) (~60%).

The phase diagram shows a region of long-range order (LRO) instead of phase separation. The LRO region is bounded by a critical composition of approximately 40% A (x ≈ 0.4). The phase diagram also shows regions of phase separation (B_x-B (30%), C₁-C₁ (20%), and C₁-C₂ (33%)) and a region of long-range order (LRO) (~60%).

II. STRAIN RELEASE THROUGH COORDINATION NUMBER DISPROPORTIONATION

The phase diagram shows a region of long-range order (LRO) instead of phase separation. The LRO region is bounded by a critical composition of approximately 40% A (x ≈ 0.4). The phase diagram also shows regions of phase separation (B_x-B (30%), C₁-C₁ (20%), and C₁-C₂ (33%)) and a region of long-range order (LRO) (~60%).

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

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

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

$$\bullet [x E_{AX}(V_{AX}) + (1-x) E_{BX}(V_{BX})]$$



The authors are grateful to the National Science Foundation (NSF) under Grant No. DE-AC36-08-28308 for providing financial support for this work. The authors also acknowledge the helpful discussions with the members of the University of California, Berkeley, Division of Energy and Geosciences.

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ACKNOWLEDGMENTS

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