

Evolution of L_{12} ordered domains in fcc Cu_3Au alloy

This content has been downloaded from IOPscience. Please scroll down to see the full text.

2007 J. Phys.: Condens. Matter 19 086201

(<http://iopscience.iop.org/0953-8984/19/8/086201>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 128.138.65.115

This content was downloaded on 14/07/2015 at 19:12

Please note that [terms and conditions apply](#).

Evolution of $L1_2$ ordered domains in fcc Cu_3Au alloy

Mahdi Sanati ¹ and Alex Zunger

Abstract

The evolution of $L1_2$ ordered domains in fcc Cu_3Au alloy is studied using a combination of Monte Carlo simulation and phase field modeling. The simulation results show that the growth of $L1_2$ domains is controlled by the interplay of surface energy and ordering energy. The phase field model captures the characteristic morphology of the domains, which grow from small nuclei and coarsen over time. The results provide insight into the kinetics of the ordering process and the role of defects in the evolution of the microstructure.

1. Introduction

The $L1_2$ ordered phase in fcc Cu_3Au alloy is a well-studied system. It exhibits a characteristic morphology of ordered domains that grow and coarsen over time. The evolution of these domains is controlled by the interplay of surface energy and ordering energy. In this work, we study the evolution of $L1_2$ ordered domains in fcc Cu_3Au alloy using a combination of Monte Carlo simulation and phase field modeling. The simulation results show that the growth of $L1_2$ domains is controlled by the interplay of surface energy and ordering energy. The phase field model captures the characteristic morphology of the domains, which grow from small nuclei and coarsen over time. The results provide insight into the kinetics of the ordering process and the role of defects in the evolution of the microstructure.

$$\langle \sigma \rangle = \langle \sigma_1 \rangle + \sum_{i=2}^{\infty} \langle \sigma_i \rangle + \sum_{i=2}^{\infty} \langle \sigma_i \rangle + \sum_{i=2}^{\infty} \langle \sigma_i \rangle + \dots$$

The evolution of the microstructure is governed by the competition between the driving force for ordering and the resistance to growth provided by surface energy. The phase field model provides a powerful tool for studying the evolution of the microstructure, as it captures the characteristic morphology of the domains and the kinetics of the ordering process. The results of this study provide a detailed understanding of the evolution of $L1_2$ ordered domains in fcc Cu_3Au alloy and the role of defects in the evolution of the microstructure.

'oo

$$(\sigma) = \sum_{\mathbf{k}} \frac{\Delta(\mathbf{k}, \sigma)}{(\mathbf{k}, \sigma)} |(\mathbf{k}, \sigma)\rangle$$

$$(\mathbf{k}) \quad \Delta(\mathbf{k}, \sigma)$$

$$(\sigma) = (\sigma) + (\sigma),$$

\pm
{ }

'oo

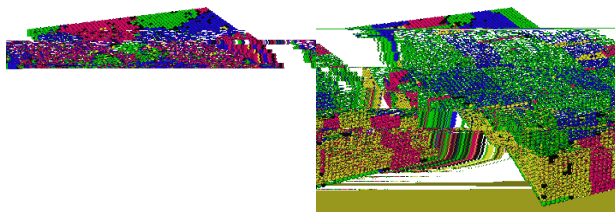
\pm

(σ)

(σ)

'oo





(a) $H_{\text{chem}} + H_{\text{strain}}$

