Evolution of $L 1_2$ ordered domains in fcc Cu₃Au 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 Cu₃Au alloy

Mahdi Sanati y and Alex Zunger

1 1// Abstract



1. Introduction

/** /)*___ '00 • $\mathbf{r} \qquad \mathbf{r} \qquad$ 100 σ $\mathbf{r} = +, , , = 1, , \dots, \mathbf{r}$ = -,, , ±



100

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

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

 (\mathbf{k},σ) $\Delta (,,\hat{})$ L (**k**) r

_

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

r 1

×



 (σ)

-









Ln[Number of MC steps (mcs)]