Prediction of alloy precipitate shapes from first principles

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U [1](*), C. [2], [3] A. [1]

1
2
3

(

PAC . 61.66.Dk A
PAC . 71.15.Mb D

PAC . 81.30.Mh -

Abstract.

A - E3N1 O0 3=1 O -

1–

$A\ B$

(

(

$A_{1-}\ B \rightleftharpoons (\ -x\ A\quad xB$

$A_{1-}\ B \rightleftharpoons A_3B\quad A$

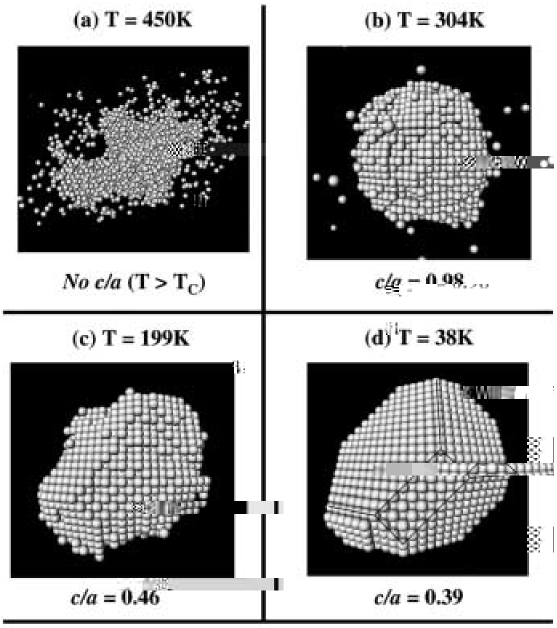
”

”

3 5

A 1–

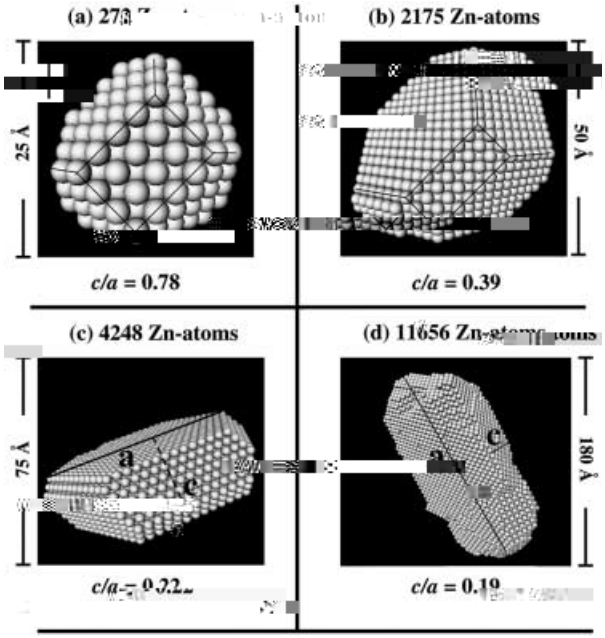
{



F . . 1 *vs.* A 24 2- 21 . O . (c/a) - (c/a) .

A $\{J_{\rm pair}(\boldsymbol{k}\}$ $\{J_f\}$ $-H_{\rm CE}(\sigma_{\rm ord}$ (A $\{\sigma_{\rm ord}\}$ (

A $-H_{\rm CE}$ $-H_{\rm LDA}$ A $\{J_{\rm pair}(\boldsymbol{k}\}$ $\{J_f\}$ —


(b) 2175 Zn-atoms
25 Å
50 Å
c/a = 0.78
c/a = 0.39
(c) 4248 Zn-atoms
75 Å
180 Å
a
c
c/a = 0.19


Mean precipitate radius r_m [

A Zn c/