Prediction of alloy precipitate shapes from first principles

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U [1](*, C. N[2], NG[3] A. UNG [1]

[1]

[2]

[3]

61.66.Dk

71.15.Mb

81.30.Mh

A B

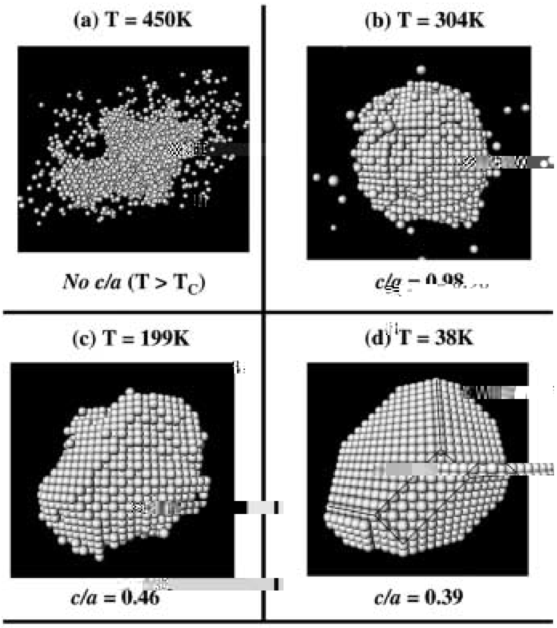
A_{1-} $B \rightleftharpoons ($ $-x$ A xB

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

3 5

A $_{1-}$

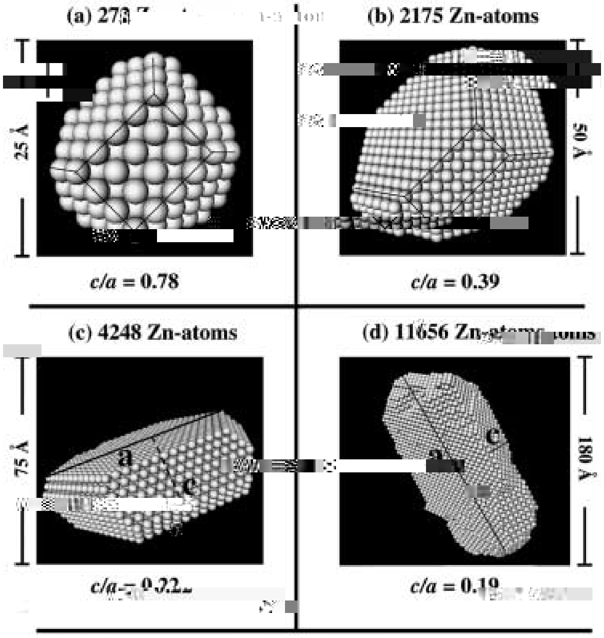
{



. 1 *vs.* 24825 2175 . , (c/a) (c/a) .

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

A , $-H_{\text{CE}}$ $-H_{\text{LDA}}$ A , $\{J_{\text{pair}}(\boldsymbol{k}\}$ $\{J_f\}$ ”


(a) 27
25 Å
c/a = 0.78
(b) 2175 Zn-atoms
50 Å
c/a = 0.39
(c) 4248 Zn-atoms
75 Å
a
c
c/a = 0.22
(d) 11656 Zn-atoms
180 Å
c
a
c/a = 0.19

Mean precipitate radius r_m [

A Zn $c/$

(