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Prediction of alloy precipitate shapes from first principles

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[illegible] **55** ([illegible] ([illegible]

P [illegible]

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

1 [illegible]

2 [illegible]

3 [illegible]

([illegible] A [illegible]

[illegible] 61.66.Dk [illegible]

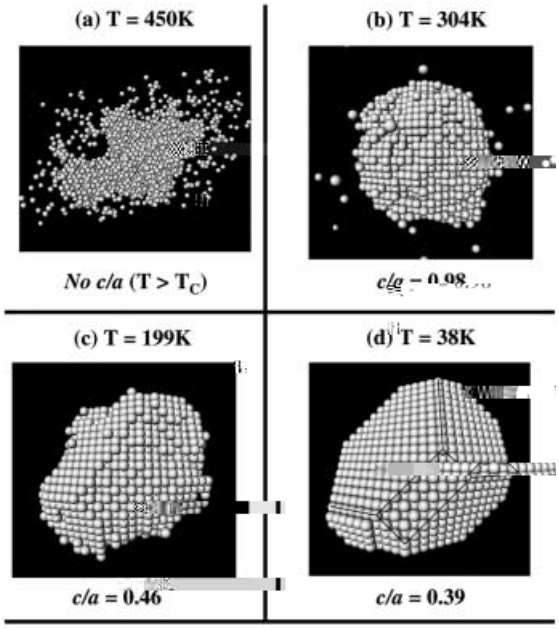
[illegible] 71.15.Mb [illegible]

[illegible] 81.30.Mh [illegible]

[illegible]

[illegible] $^{1-}$ [illegible] A B [illegible] A_{1-} B $\rightleftharpoons$ ($-x$ A xB [illegible] A_{1-} B $\rightleftharpoons$ A_3B A [illegible] ” [illegible] ” [illegible] ^{3} ^{5} [illegible] A $_{1-}$ [illegible]

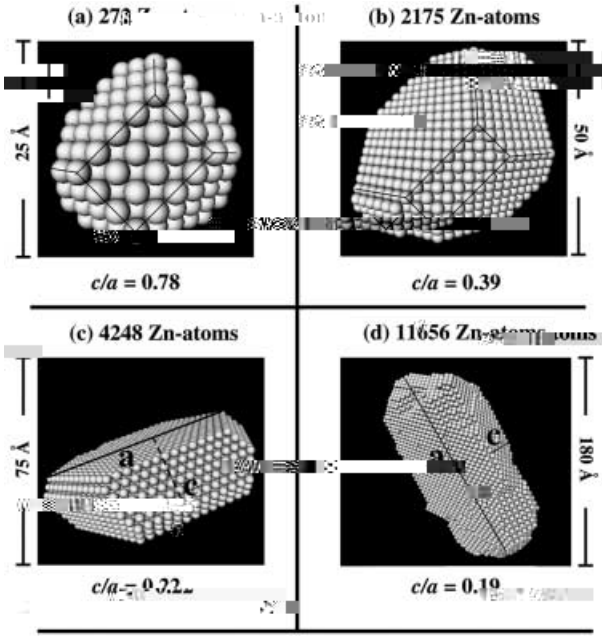
{ [illegible]



0 . 1 , — vs. . — . — . 0.0 0 24825 2175— . — . — . 0 — 0 . , — — . — — . 0 (c/a) — . — - 0 (— c/a) . .

A

. {$J_{\mathrm{pair}}(\boldsymbol{k}$ } {J_f} . . . $-H_{\mathrm{CE}}$(ȯrd . . . . (A , . . . { ȯrd} (, , . . . , , ... , , ,


(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/