

Prediction of alloy precipitate shapes from first principles

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P

U¹(*, C. N², A. U_NG³ 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

(A B
 (A₁- B ⇒ (-x A xB
 A₁- B ⇒ A₃B A
 3 5
 A₁-

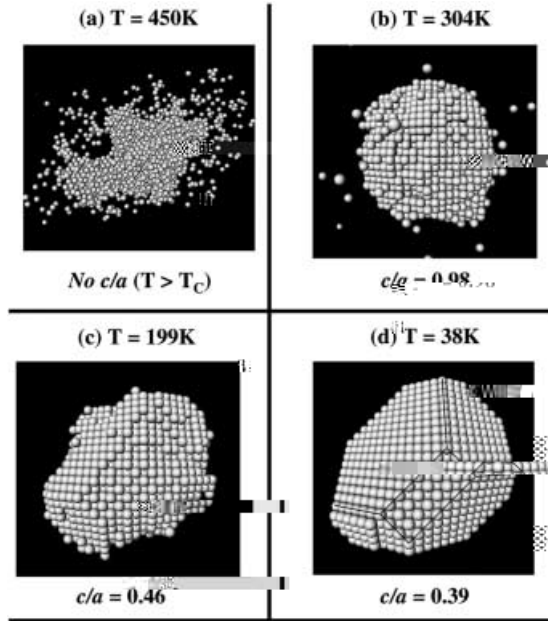
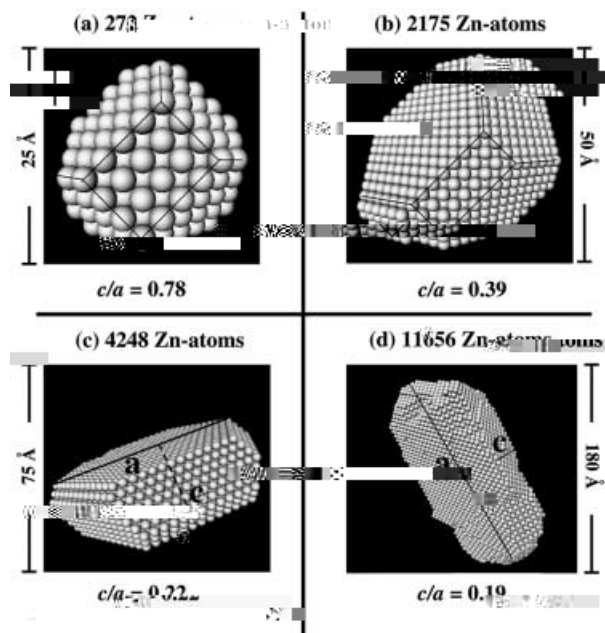


FIG. 1. Evolution of the crystal structure of $\text{A}_{24}\text{Zr}_{21}\text{O}_{51}$ as a function of temperature (O: oxygen, Zr: zirconium, A: yttrium) and the c/a ratio.

$$\begin{aligned}
 & \mathbf{A} \left(\begin{array}{c} \{J_{\text{pair}}(\mathbf{k})\} \\ \{J_f\} \end{array} \right) - H_{\text{CE}}(\{\text{ord}\}) \quad \mathbf{A} \left(\begin{array}{c} \{J_{\text{pair}}(\mathbf{k})\} \\ \{J_f\} \end{array} \right) - H_{\text{LDA}}(\{\text{ord}\}) \\
 & \mathbf{A} \left(\begin{array}{c} \{J_{\text{pair}}(\mathbf{k})\} \\ \{J_f\} \end{array} \right) - H_{\text{CE}}(\{\text{ord}\}) \quad \mathbf{A} \left(\begin{array}{c} \{J_{\text{pair}}(\mathbf{k})\} \\ \{J_f\} \end{array} \right) - H_{\text{LDA}}(\{\text{ord}\})
 \end{aligned}$$



Mean precipitate radius r_m [

A \dots Zn \dots $c/$ \dots