First-principles kinetic theory of precipitate evolution in Al-Zn alloys

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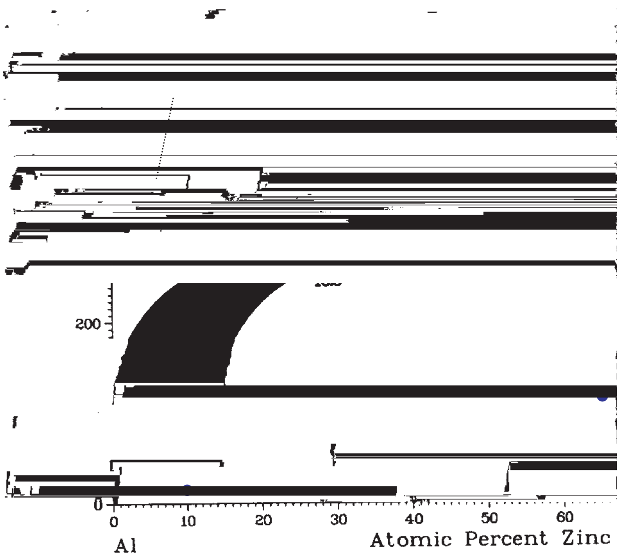

200
0
0
10
20
30
40
50
60
Al
Atomic Percent Zinc

(...) 21 . (.) (..) W (...) 1/

2. t

2.1. Cluster expansion of substitutional configurational energies

T E (σ) ( ) 21 . σ N (-1) ($+1$). T σ

$$\Delta H \quad (\sigma) \quad \sum_{\boldsymbol{k}} J(\boldsymbol{k}) \quad (\boldsymbol{k},\sigma)^2 + \sum D \quad J \quad \Pi \quad (\sigma) + \frac{1}{\quad - 1} \sum_{\boldsymbol{k}} \Delta E \; (\; , \;) \quad (\boldsymbol{k},\sigma)^2. \tag{1}$$

T 2 . $J(\boldsymbol{k})$ $(\boldsymbol{k},\sigma)$ T ( ) J , D Π (σ) T (1) ( ) W (1) *atomistically* (W) $J(\boldsymbol{k})$ J H

(1). ( ) ( ) $1/\tau_0$, D ( )

$$\tau_0( ) \quad \frac{2}{D\ ( )}, \tag{2}$$

-1, $+1$. T without destroying the Markovian process. T

1. N
2. each N ($12N$,).

$\delta E(\ )$ each ($1, \ldots,$).

$\delta E(\ ) > 0$, $(1/\tau_0)$ $(-\delta E(\ )/\ )$. $\delta E(\ ) < 0$, $1/\tau_0$.

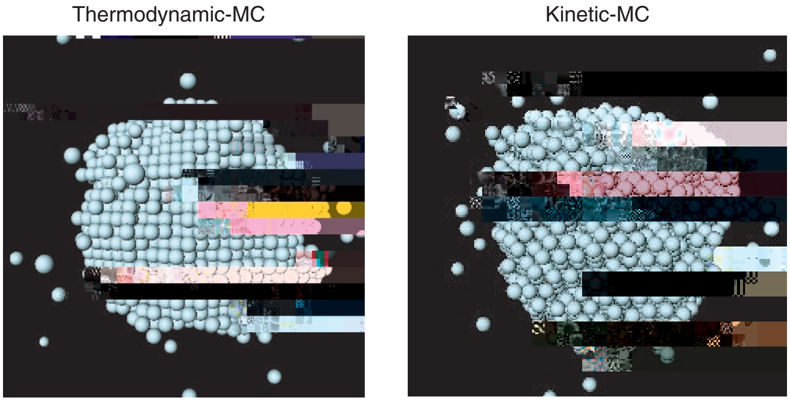
P / , $\sum_1$.

P. $_{-1} + 1/$ ($\sum_1$ not .')

$\delta E(\ )$'.

T $\delta E(\ )$' ( ) $(\boldsymbol{k}, \sigma)$ (1). et al 2 , $(\boldsymbol{k}, \sigma)$ change $J(\boldsymbol{k})$ $(\boldsymbol{k}, \sigma)$ 2 2 . T no longer a constant real time unit, 1/1000 1 .

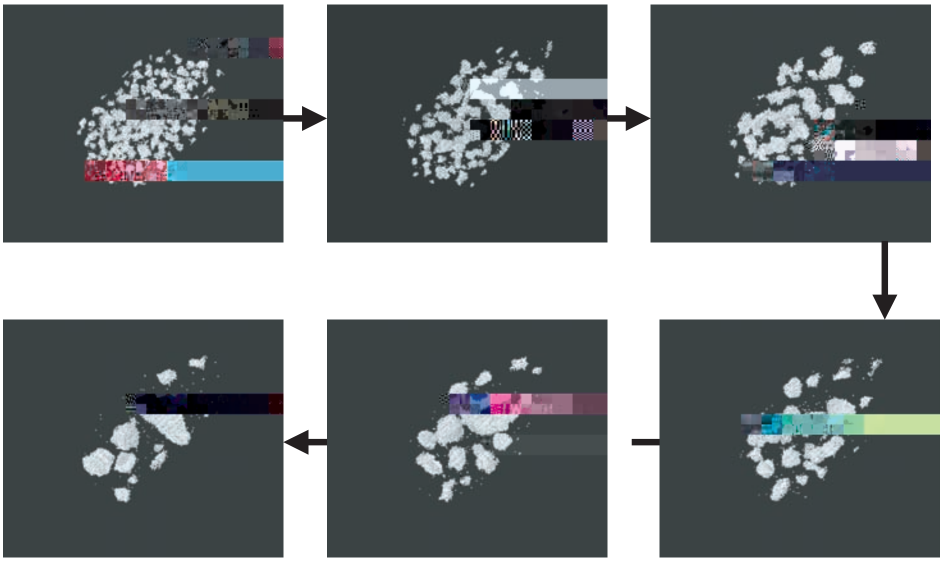
not (. 1000 1 000), -1, T ' 11 , et al , T (. 1).

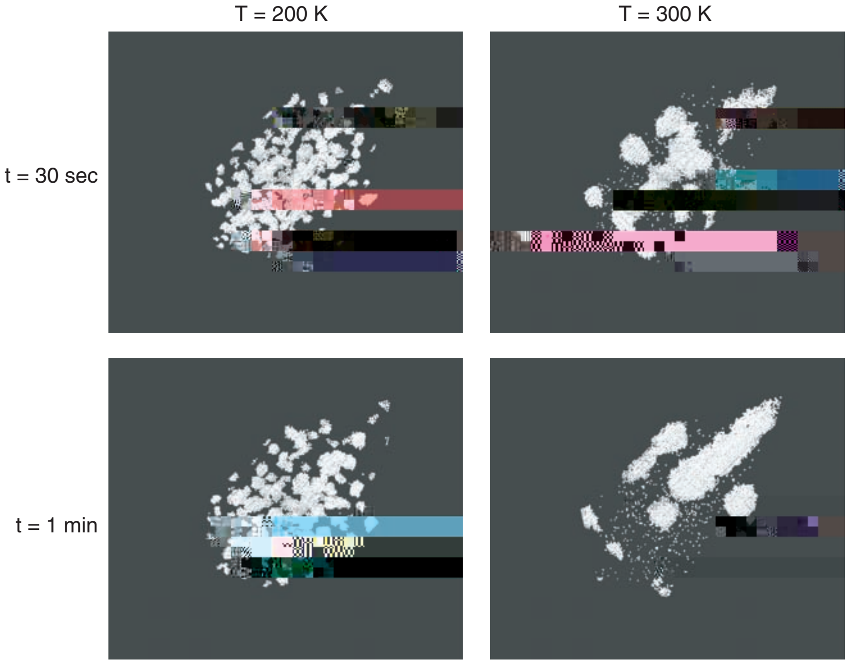


2. ... 0. 2 ... 0.0 ...).

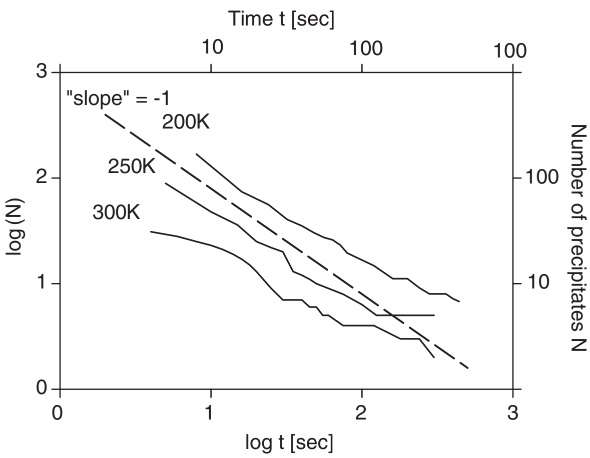
1. (4)) 0. 2 0.0 (00) T 2.

( )	α	α
000	1.000	1.000
110	0.	0. 00
200	0.	0. 2
211	0. 1	0. 01
220	0. 0	0.
10	0.	0.
222	0.	0. 1
21	0. 2	0. 11
4 00	0. 1	0. 0
0	0.	0.
4 11	0. 02	0.



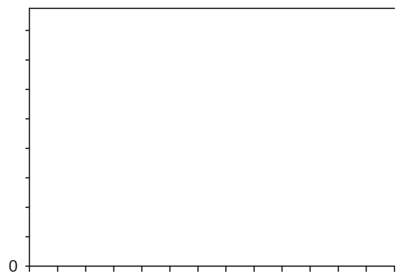


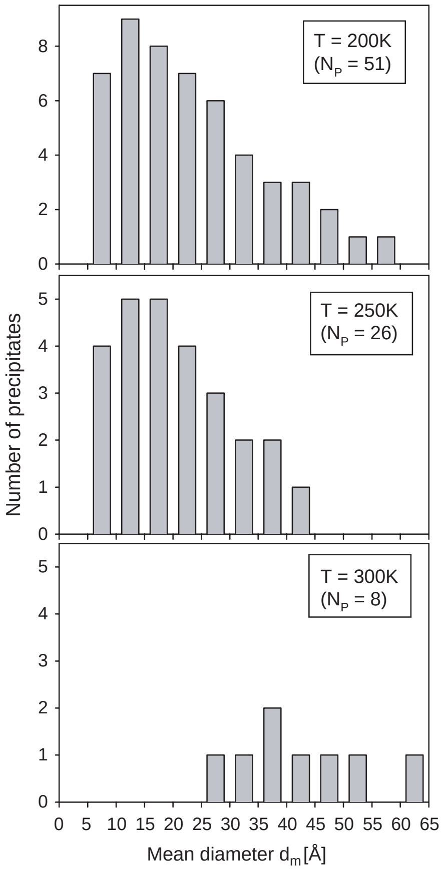
[illegible] 4. [illegible] ([illegible]).



[illegible] 5. [illegible] 0. [illegible] 2 [illegible] 0.0 [illegible] (11.4 2 [illegible]) [illegible] T [illegible] −1, [illegible] (- - - -).

[illegible] T [illegible] 2 0 [illegible], [illegible] 2 0 [illegible] [illegible]





[illegible] (0).

4. [illegible]

T[illegible] ( ) [illegible] W [illegible] ( ).

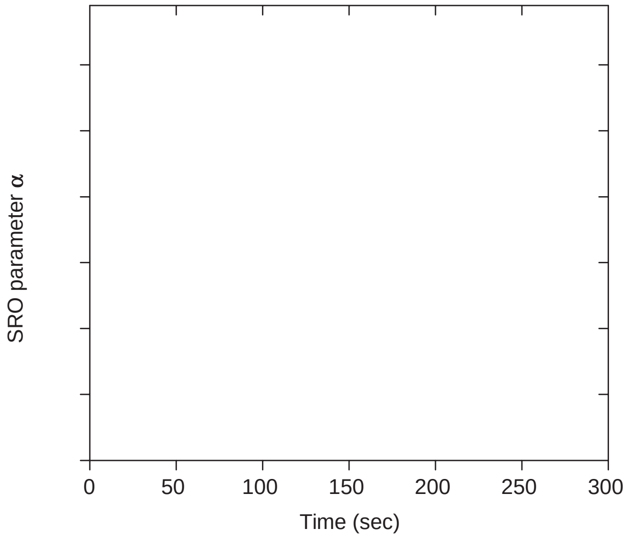
$$\alpha \quad ( ) \quad 1 - \frac{P^{A(B)}}{\quad},$$ ( )

[illegible] $P^{A(B)}$ [illegible] A [illegible] B [illegible] ( ). T[illegible] α [illegible] $(\alpha < 0)$ [illegible] $(\alpha > 0)$. T[illegible]

$$\alpha \quad ( ) \quad \frac{\Pi \quad - \quad ^2}{1 - \quad ^2},$$ (4)

[illegible] 2 − 1 [illegible] Π [illegible] ( ). [illegible] α ( ).

$$\alpha(\, , \boldsymbol{k}) \quad \sum^{R} \alpha \quad ( ) \, \cdot \boldsymbol{k} \cdot \boldsymbol{R} \; .$$ ( )


SRO parameter α
0
50
100
150
200
250
300
Time (sec)

1 W Y, [illegible] 1 1 *Scripta Metall.*