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

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[illegible] **10** (2002) 1 1 4 [illegible] 0 -0 (02) 0 2-

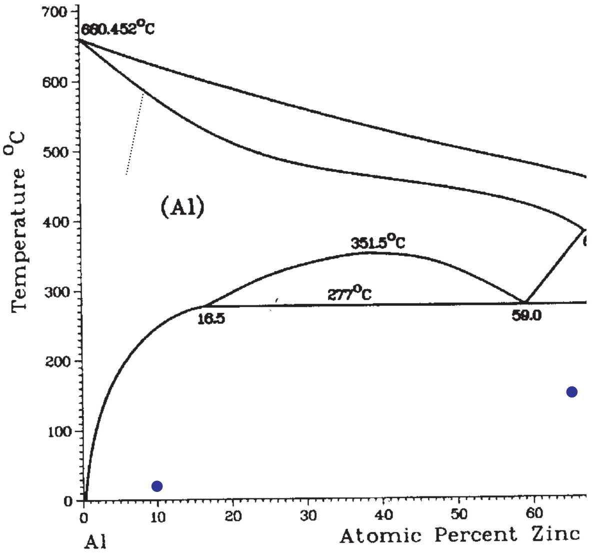
[illegible]

[illegible][1], [illegible][2] [illegible][1]

[1] [illegible] 01,
[2] [illegible] 4 20,

[illegible]

[illegible] 20 [illegible] 2001
[illegible] 2002
[illegible]


700
600
500
400
300
200
100
0
Temperature °C
660.452°C
(Al)
351.5°C
277°C
16.5
59.0
0
10
20
30
40
50
60
Al
Atomic Percent Zinc

(...) 21 . , ( ) , ( ) (...) 1/

2. t

2.1. Cluster expansion of substitutional configurational energies

T E (σ) ( ) 21 . σ N (-1). ($+1$). T σ

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

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

[illegible] (1). [illegible] $1/\tau_0$, [illegible] D [illegible]

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

[illegible]

[illegible] -1, [illegible] $+1$. T[illegible] *without destroying the Markovian process.* T[illegible]

1. [illegible] N [illegible]
2. [illegible] *each* [illegible] N [illegible] ([illegible] $12N$, [illegible]).

[illegible] $\delta E(\ )$ [illegible] *each* [illegible] ([illegible] $1, \ldots,$ [illegible]).

4 [illegible] $\delta E(\ ) > 0$, [illegible] $(1/\tau_0)$ [illegible] $(-\delta E(\ )/\ )$. [illegible] $\delta E(\ ) < 0$, [illegible] $1/\tau_0$.

[illegible] P [illegible] $/$ [illegible] $\sum$ [illegible] 1 [illegible]

[illegible] P.

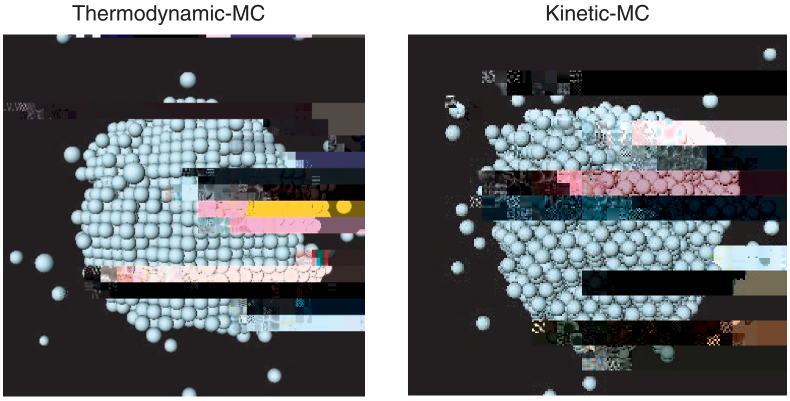
[illegible] $_{-1} + 1/$ [illegible] ([illegible] $\sum$ 1 [illegible] *not* [illegible] ’.)

[illegible] $\delta E(\ )$’.

[illegible] 4 .

T[illegible] $\delta E(\ )$’ ([illegible]) [illegible] $(\boldsymbol{k}, \sigma)$ [illegible] (1). [illegible] *et al* [illegible] 2 , [illegible] $(\boldsymbol{k}, \sigma)$ [illegible] *change* [illegible] J [illegible] $(\boldsymbol{k})$ $(\boldsymbol{k}, \sigma)$ 2 [illegible] 2 [illegible] T[illegible] 4 [illegible] *no longer a constant real time unit,* [illegible] 1/1000 [illegible] 1 .

[illegible] *not* [illegible] ([illegible] 1000 1 000), [illegible] -1, [illegible] T[illegible] ’ 11 , [illegible] *et al* [illegible] , [illegible] T[illegible] ([illegible] 1). [illegible]

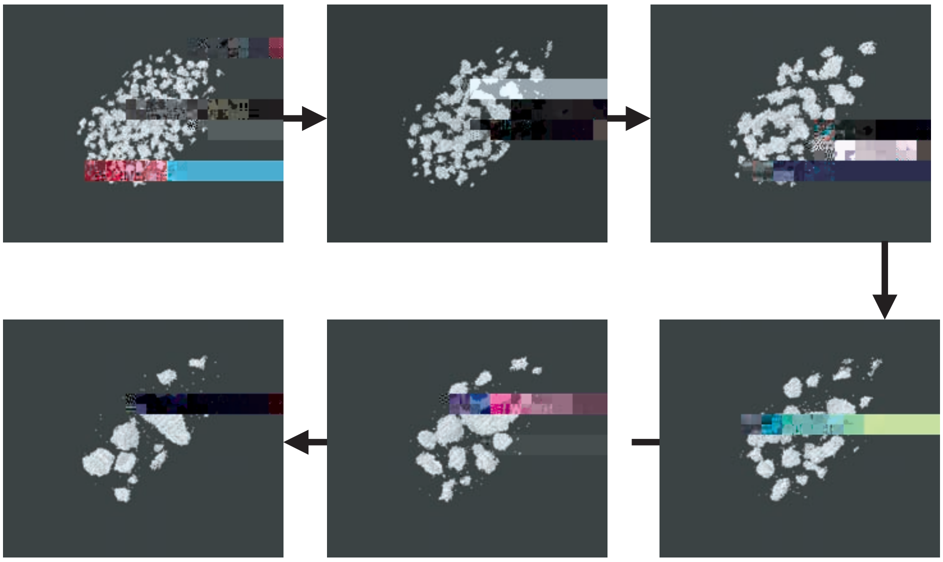


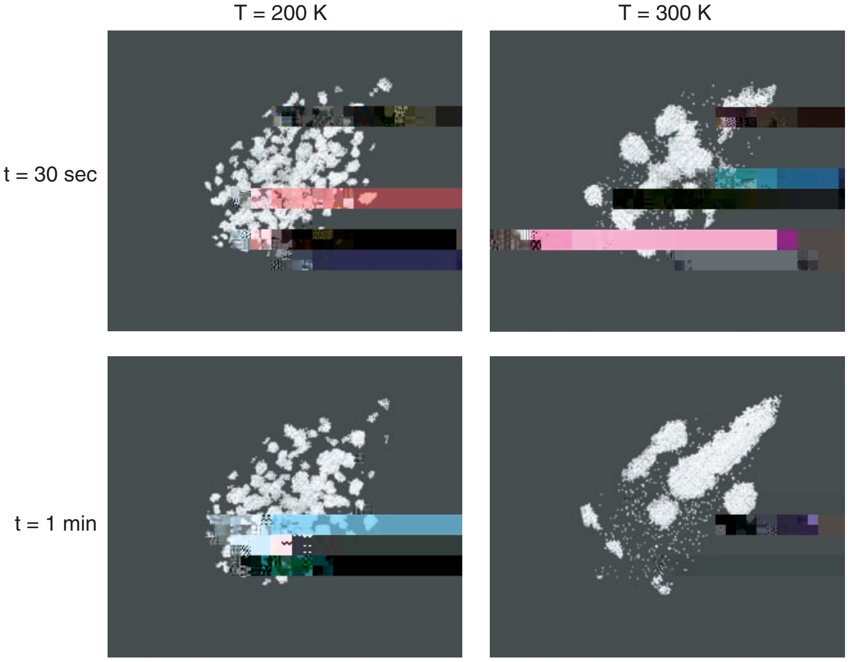
[illegible] 2. [illegible] 0. 2 [illegible] 0.0 [illegible] ([illegible]).

[illegible]

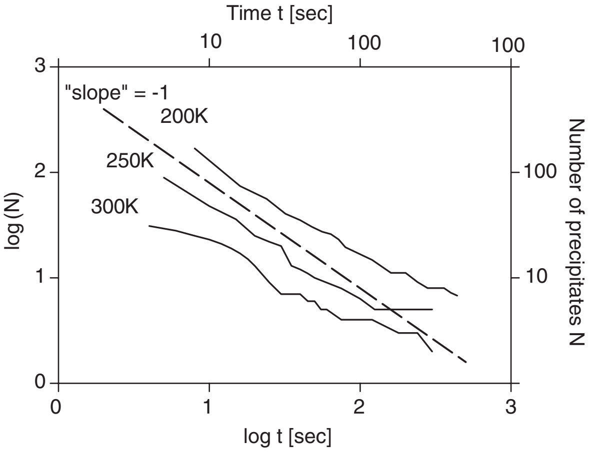
1. [illegible] ([illegible] 4)) [illegible] 0. 2 [illegible] 0.0 [illegible] ([illegible] 00) [illegible]. T[illegible] 2.

([illegible])	α[illegible]	α[illegible]
000	1.000	1.000
110	0.[illegible]0	0.[illegible]00
200	0.4[illegible]	0.[illegible]2
211	0.[illegible]1	0.[illegible]01
220	0.[illegible]0	0.[illegible]
[illegible]10	0.[illegible]	0.[illegible]
222	0.[illegible]	0.[illegible]1
[illegible]21	0.[illegible]2	0.[illegible]11
4[illegible]00	0.[illegible]1	0.[illegible]0
[illegible]0	0[illegible]	0[illegible]
4[illegible]11	0.[illegible]02	0[illegible]



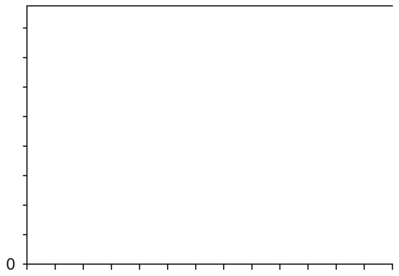


[illegible] 4. [illegible] ([illegible]).



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

[illegible] T [illegible] 2 0 [illegible], [illegible] 2 0 . [illegible], [illegible]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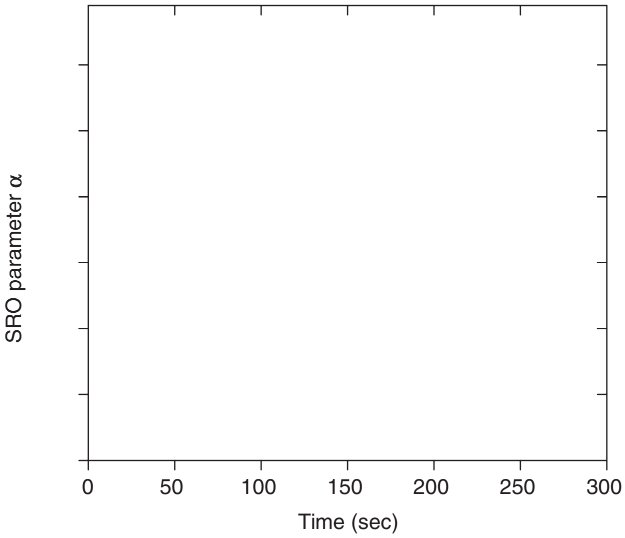
SRO parameter α
0
50
100
150
200
250
300
Time (sec)

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