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

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(http://iopscience.iop.org/0965-0393/10/2/303)

. 10 (2002) 1 1 4 0 -0 (02) 0 2-

t t t y

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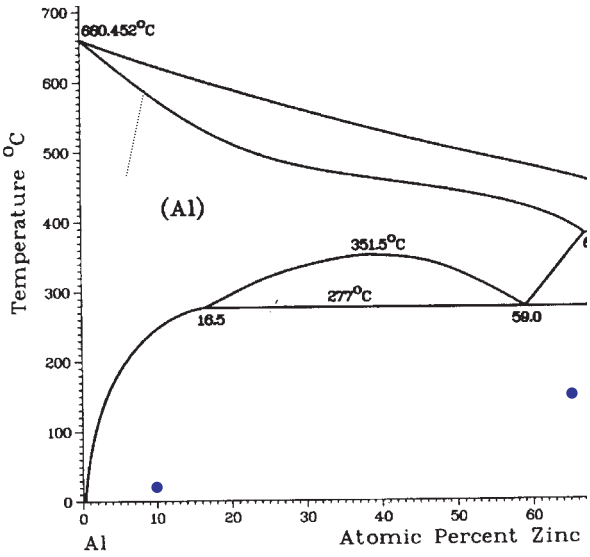

660.452°C
(Al)
351.5°C
277°C
16.5
59.0
Temperature °C
700
600
500
400
300
200
100
0
0
10
20
30
40
50
60
Al
Atomic Percent Zinc

1/

2. t

2.1. Cluster expansion of substitutional configurational energies

$$\Delta H(\sigma) \approx \sum_{\boldsymbol{k}} J(\boldsymbol{k})\, |(\boldsymbol{k},\sigma)|^2 + \sum D\, J\, \Pi(\sigma) + \frac{1}{4(N-1)} \sum_{\boldsymbol{k}} \Delta E(\,,\,)\, |(\boldsymbol{k},\sigma)|^2. \tag{1}$$

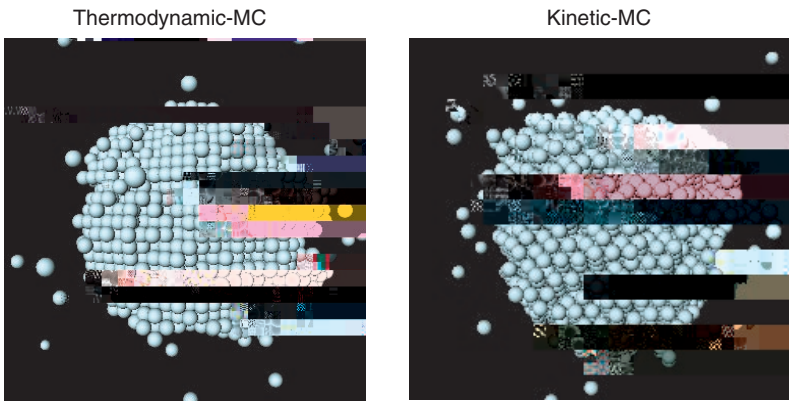
atomistically

(1). ( ) ( ) , $1/\tau_0$, $D_{\_}( )$

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

without destroying the Markovian process.

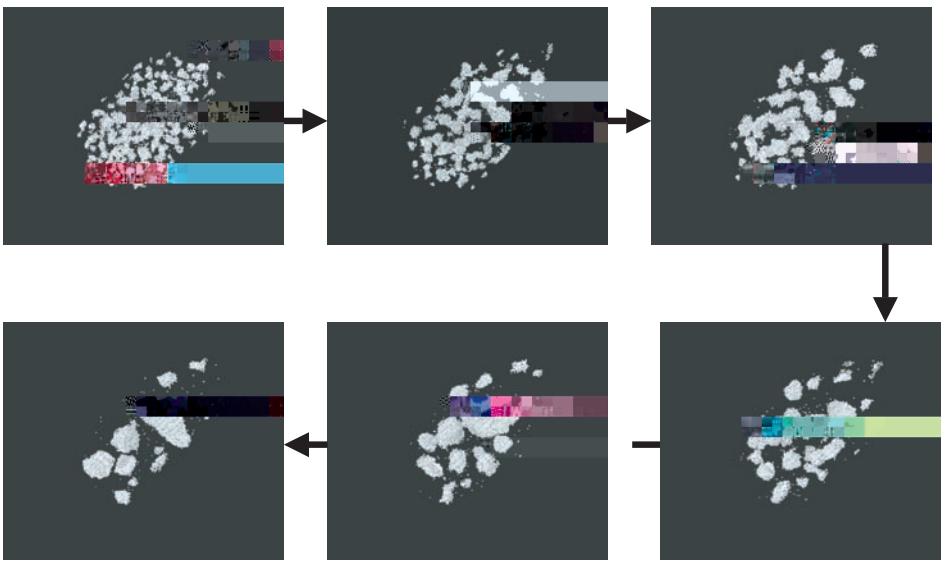
1.
2. *each*
4
4

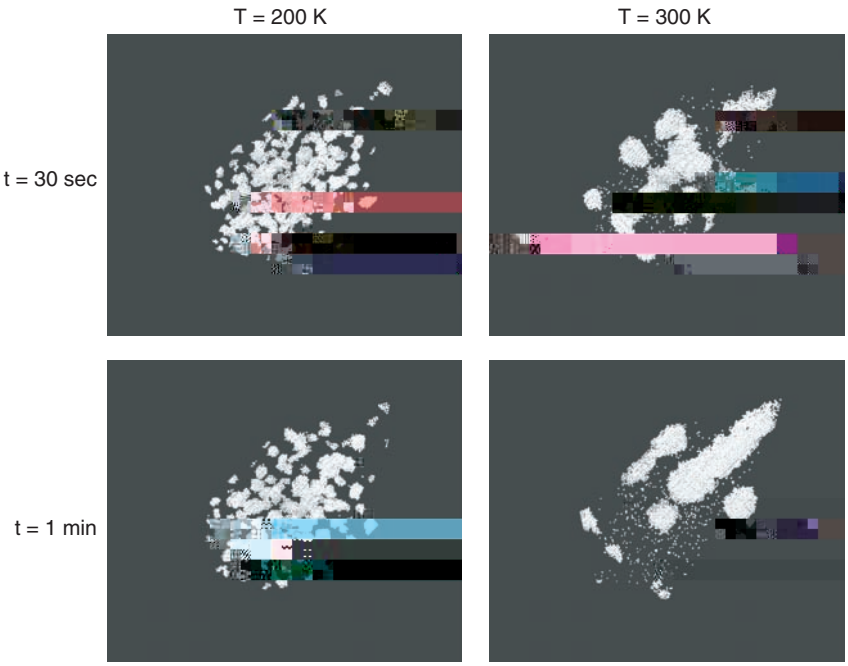


2. 0. 2 0.0 ( ).

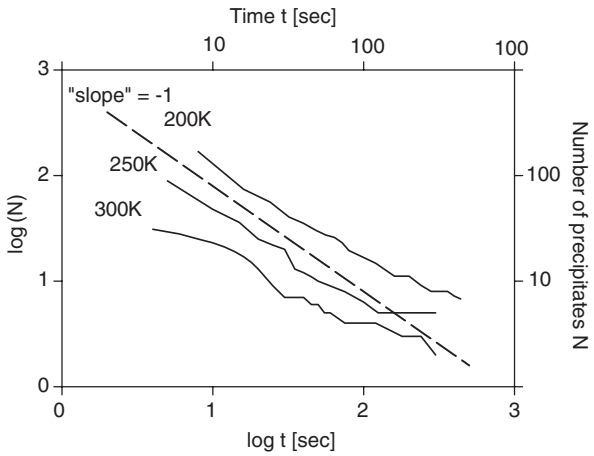
1. (4)) 0. 2 0.0 (00) . T 2.

( )	α	α
000	1.000	1.000
110	0. 0	0. 00
200	0.4	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



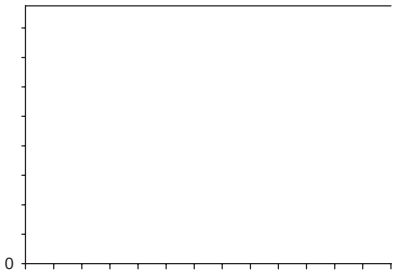


۴ 4. . . . . . (. . . . .).



۴ 5. . . . . . 0. 2 . 0.0 . . . (11.4 2 . . . . .) . . . . . T . . . . . −1, ... (- - - -).

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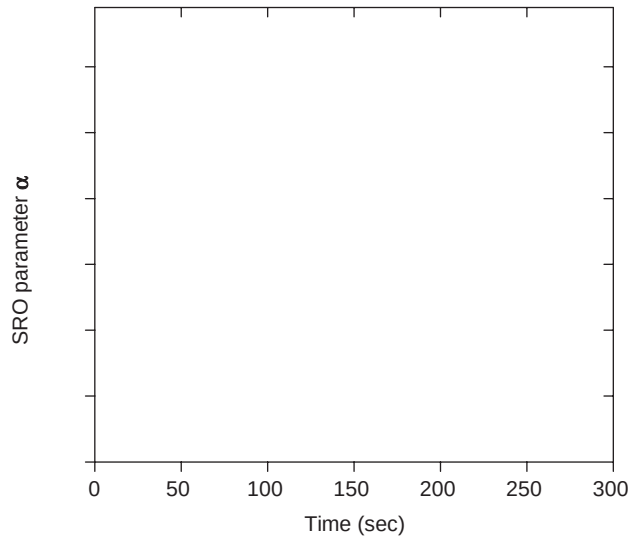
SRO parameter α
0
50
100
150
200
250
300
Time (sec)

1 W Y 1 1 *Scripta Metall.*