

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

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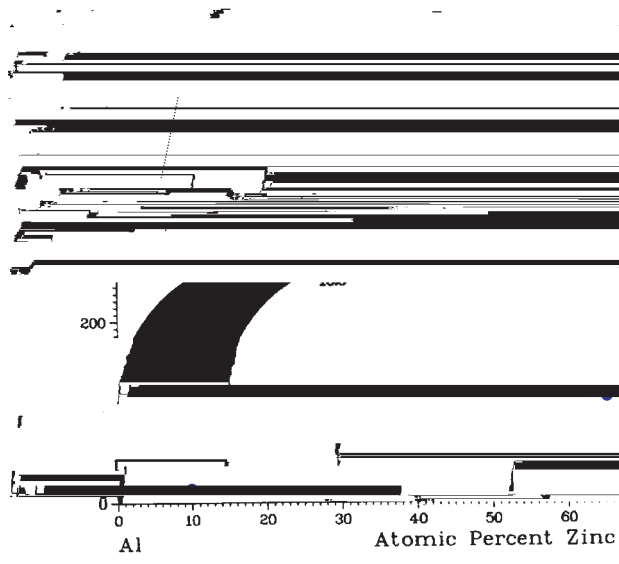
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$\tau_0(\omega) = \frac{1}{D_{\text{eff}}(\omega)}$ (1). (2) The effective diffusion coefficient $D_{\text{eff}}(\omega)$ is defined as the inverse of the sum of the inverse of the diffusion coefficient D_0 and the inverse of the relaxation time τ_0 , i.e. $\frac{1}{D_{\text{eff}}(\omega)} = \frac{1}{D_0} + \frac{1}{\tau_0}$.

$$\tau_0(\omega) = \frac{2}{D_{\text{eff}}(\omega)}, \quad (2)$$

without destroying the Markovian process. \mathbb{T}

1. N
 2. N each N ($1, \dots, N$).
 3. $\delta E(i)$ each ($1, \dots, N$).
 4. $\delta E(i) > 0$, $(1/\tau_0)$, $(-\delta E(i)/\tau_0)$, $\delta E(i) < 0$, $1/\tau_0$.
- P / $\sum_{i=1}^N 1$ P .
- $\sum_{i=1}^N$ not $-1 + 1/$ ($\delta E(i)$) $\delta E(i)$.
- 4.

\mathbb{T} $\delta E(i)$ ($1, \dots, N$) *et al* 2, (\mathbf{k}, σ) *change* $J_{\mathbf{k}}(\mathbf{k}, \sigma)^2$ 2. \mathbb{T} *no longer a constant real time unit*, $1/1000$.

not ($1, 1000$ 1 000), -1 , \mathbb{T} 11, *et al* \mathbb{T} (1).

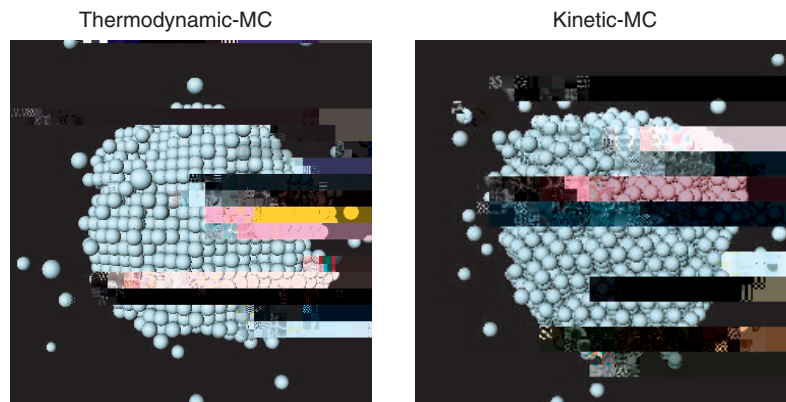
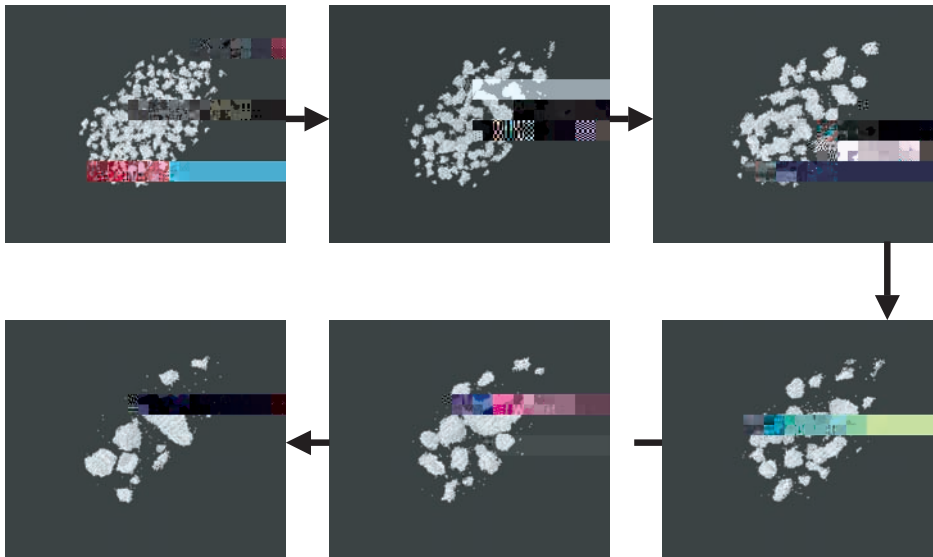


Fig. 2. Snapshots of the simulation of the cluster of Mn^{2+} ions ($0.2 \pm 0.0 \mu\text{m}$) in solution at $T = 300 \text{ K}$ and $p = 1 \text{ bar}$ (left) and $T = 300 \text{ K}$ and $p = 1 \text{ bar}$ (right).

The simulation was performed using the GROMACS software package (GROMACS, 2013).

Table 4: α values for the α parameter in the α -stable distribution (see Section 4) for $\alpha = 0.2, 0.0$ and $\alpha = 0.00$ (see Section 4) for the α -stable distribution. The α values are given in the α -stable distribution (see Section 4).

()	$\alpha = 0.2$	$\alpha = 0.0$
000	1.000	1.000
110	0.4	0.00
200	0.4	0.2
211	0.1	0.01
220	0.0	0.0
10	0.0	0.0
222	0.0	0.1
21	0.2	0.11
4 00	0.1	0.0
0	0.0	0.0
4 11	0.02	0.0



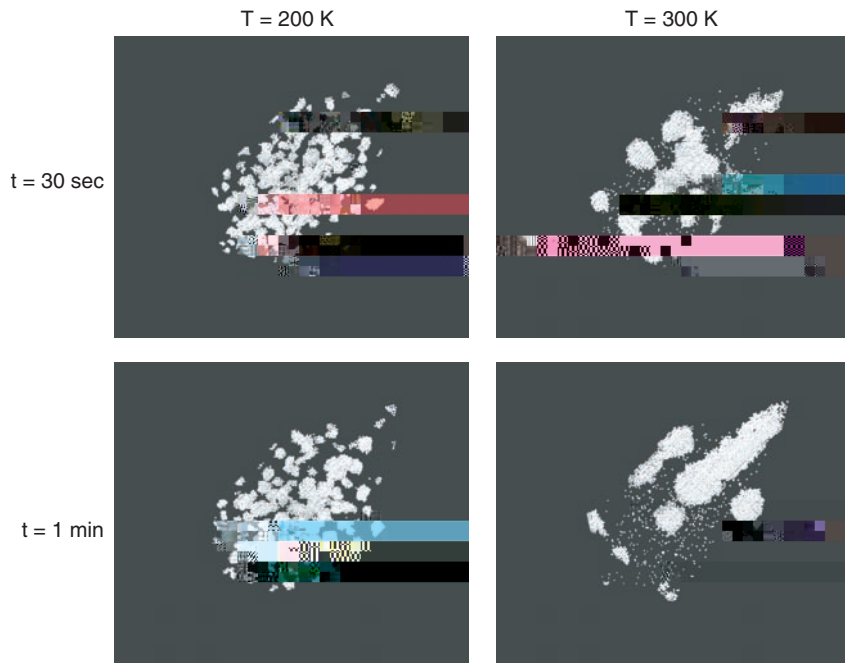


Fig. 4. Morphology of precipitates at different temperatures and times. The images are taken from the simulation at $T = 200$ K (left column) and $T = 300$ K (right column) at $t = 30$ sec (top row) and $t = 1$ min (bottom row).

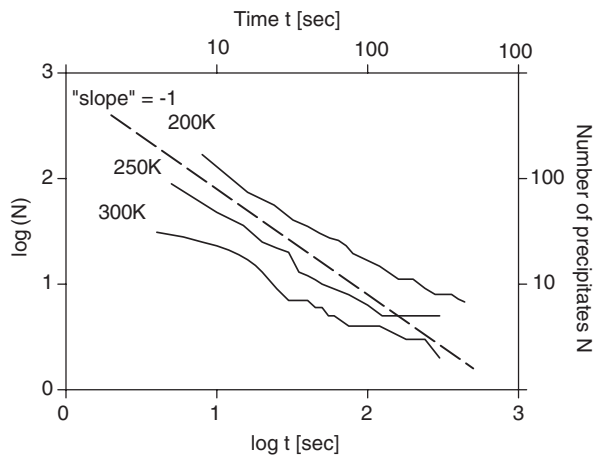
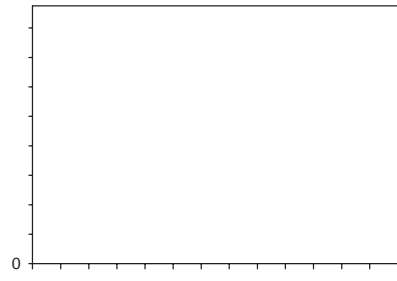


Fig. 5. The number of precipitates N versus time t [sec] for different temperatures $T = 200, 250, 300$ K. The solid lines represent the data, and the dashed line represents the fit with a slope of -1 .

The number of precipitates N versus time t [sec] for different temperatures $T = 200, 250, 300$ K. The solid lines represent the data, and the dashed line represents the fit with a slope of -1 . The number of precipitates decreases over time for all temperatures, with the rate of decrease being similar across the different temperatures.



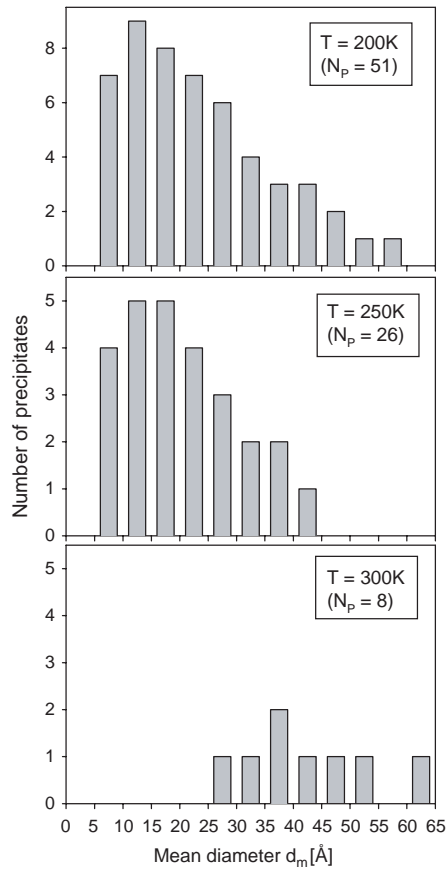


Fig. 4.1. Number of precipitates versus mean diameter of precipitates ($\alpha = 0$).

4.

The number of precipitates (N_p) versus mean diameter of precipitates (d_m) is given by the following equation:

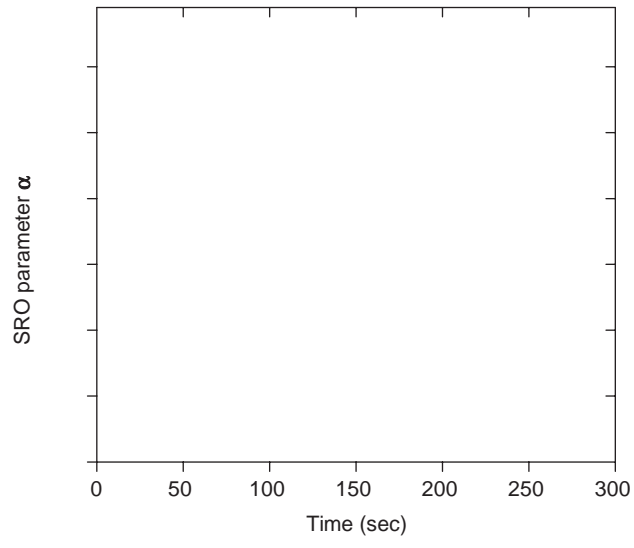
$$\alpha(d_m) = 1 - \frac{P^{A(B)}}{W}, \quad (4.1)$$

where $P^{A(B)}$ is the probability of precipitation of precipitates A and B respectively ($\alpha < 0$), $\alpha > 0$ is the probability of precipitation of precipitates A and B respectively ($\alpha < 0$), $\alpha > 0$ is the probability of precipitation of precipitates A and B respectively ($\alpha < 0$).

$$\alpha(d_m) = \frac{\Pi - 2}{1 - 2}, \quad (4.2)$$

where $\Pi = 2 - 1$ and Π is the probability of precipitation of precipitates A and B respectively ($\alpha < 0$).

$$\alpha(d_m, k) = \sum_{R=1}^R \alpha(d_m) \cdot k \cdot R, \quad (4.3)$$



1. $\int_{-\infty}^{\infty} \delta(x) dx = 1$ *Scripta Metall.*