

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

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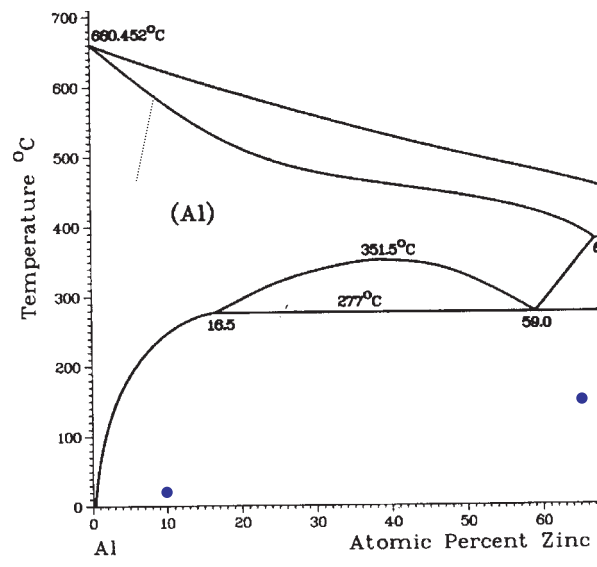
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\mathbf{W}_i is the i -th component of the vector \mathbf{W} and $\mathbf{W}_i = \mathbf{W} \cdot \mathbf{e}_i$, where \mathbf{e}_i is the i -th unit vector. The vector \mathbf{W} is defined by the equation $\mathbf{W} = \frac{1}{N} \sum_{\mathbf{k}} \mathbf{W}(\mathbf{k})$, where $\mathbf{W}(\mathbf{k})$ is the vector of the \mathbf{k} -th component of the vector \mathbf{W} . The vector \mathbf{W} is defined by the equation $\mathbf{W} = \frac{1}{N} \sum_{\mathbf{k}} \mathbf{W}(\mathbf{k})$, where $\mathbf{W}(\mathbf{k})$ is the vector of the \mathbf{k} -th component of the vector \mathbf{W} .

2. t

2.1. Cluster expansion of substitutional configurational energies

The total energy $E(\sigma)$ of a system of N atoms is a function of the configuration σ of the atoms. The total energy $E(\sigma)$ can be written as $E(\sigma) = \sum_{\mathbf{k}} J_{\mathbf{k}}(\sigma) + \sum_{\mathbf{k}} D_{\mathbf{k}} \Pi(\sigma) + \frac{1}{4} \frac{1}{-1} \sum_{\mathbf{k}} \Delta E_{\mathbf{k}}(\sigma) (\mathbf{k}, \sigma)^2$.

$$\Delta H_{\mathbf{k}}(\sigma) = \sum_{\mathbf{k}} J_{\mathbf{k}}(\mathbf{k}, \sigma)^2 + \sum_{\mathbf{k}} D_{\mathbf{k}} J_{\mathbf{k}} \Pi(\sigma) + \frac{1}{4} \frac{1}{-1} \sum_{\mathbf{k}} \Delta E_{\mathbf{k}}(\sigma) (\mathbf{k}, \sigma)^2. \quad (1)$$

The total energy $E(\sigma)$ of a system of N atoms is a function of the configuration σ of the atoms. The total energy $E(\sigma)$ can be written as $E(\sigma) = \sum_{\mathbf{k}} J_{\mathbf{k}}(\sigma) + \sum_{\mathbf{k}} D_{\mathbf{k}} \Pi(\sigma) + \frac{1}{4} \frac{1}{-1} \sum_{\mathbf{k}} \Delta E_{\mathbf{k}}(\sigma) (\mathbf{k}, \sigma)^2$. The vector \mathbf{W} is defined by the equation $\mathbf{W} = \frac{1}{N} \sum_{\mathbf{k}} \mathbf{W}(\mathbf{k})$, where $\mathbf{W}(\mathbf{k})$ is the vector of the \mathbf{k} -th component of the vector \mathbf{W} . The vector \mathbf{W} is defined by the equation $\mathbf{W} = \frac{1}{N} \sum_{\mathbf{k}} \mathbf{W}(\mathbf{k})$, where $\mathbf{W}(\mathbf{k})$ is the vector of the \mathbf{k} -th component of the vector \mathbf{W} .

$\tau_0(\omega) = \frac{1}{D_{\text{eff}}(\omega)}$ (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 / $\sum_{i=1}^N P$
- $\sum_{i=1}^N$ not $-1 + 1/$ ($\delta E(i)$)
- $\delta E(i)$.
- 4.

\mathbb{T} $\delta E(i)$ ($1, \dots, N$) *et al* 2, (\mathbf{k}, σ) (\mathbf{k}, σ) change $J_{\mathbf{k}}(\mathbf{k}, \sigma)^2$ 2. \mathbb{T} 4 *no longer a constant real time unit*, $1/1000$.

not ($1, 1000 \dots 1000$), -1 .

\mathbb{T} 11, *et al* \mathbb{T} ($1, \dots, N$).

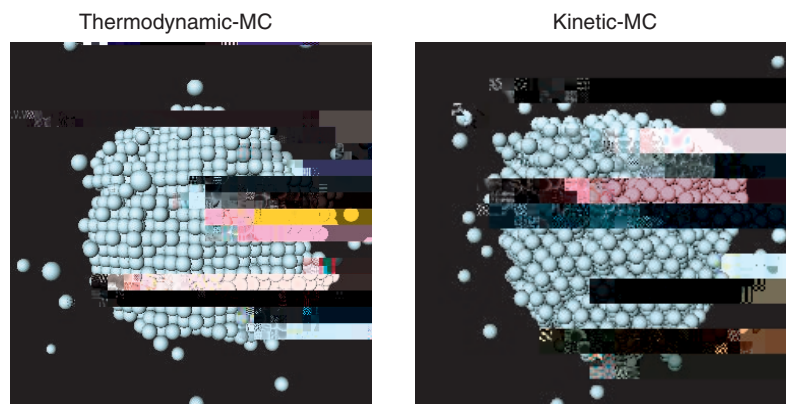
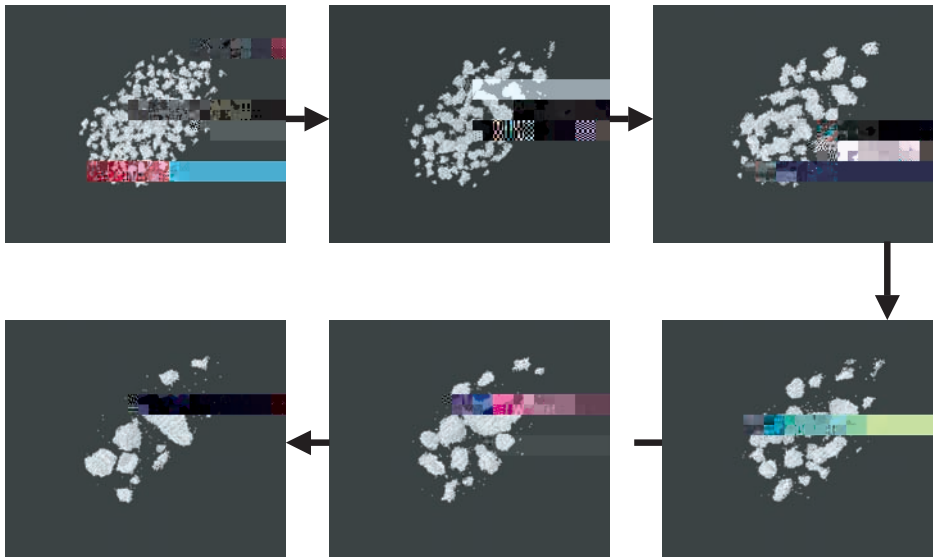


Fig. 2. Snapshots of the simulation of a cluster of $M = 1000$ particles ($\mu = 0.2 - 0.0$) in a solution of $\mu = 0.2 - 0.0$ particles (yellow and red spheres) at $T = 0.2$ (left) and $T = 0.4$ (right).

At $T = 0.2$, the cluster is stable and the particles are arranged in a compact structure. At $T = 0.4$, the cluster is more dynamic and the particles are more dispersed.

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



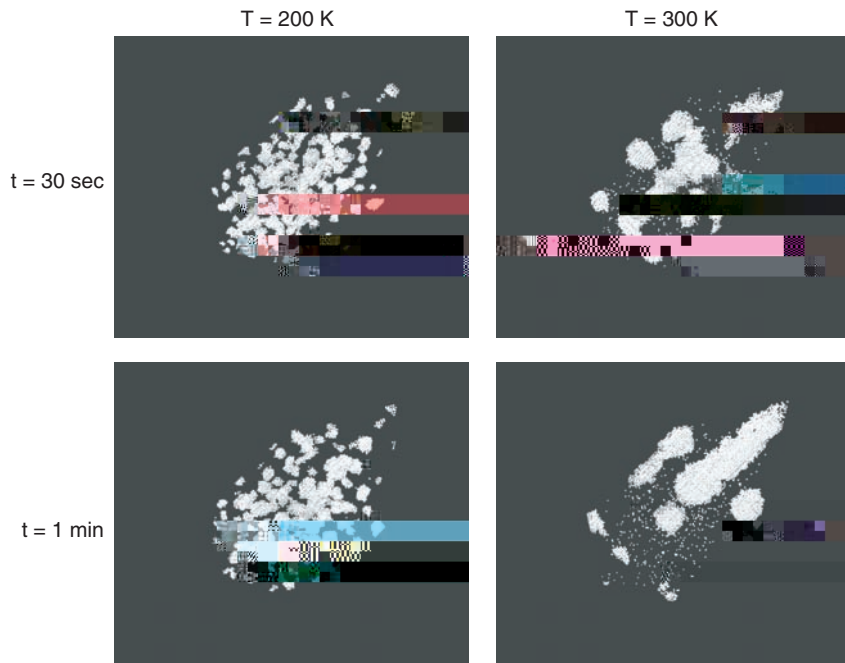


Fig. 4. Morphology of precipitates at different temperatures and times. The images are taken from the simulation at $T = 200$ K (left column) and $T = 300$ K (right column) at $t = 30$ sec (top row) and $t = 1$ min (bottom row).

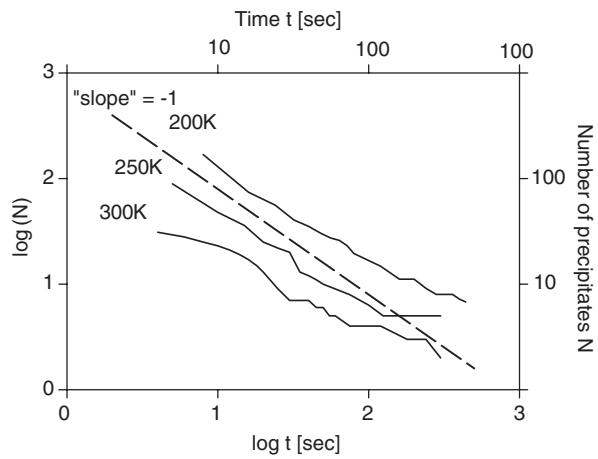
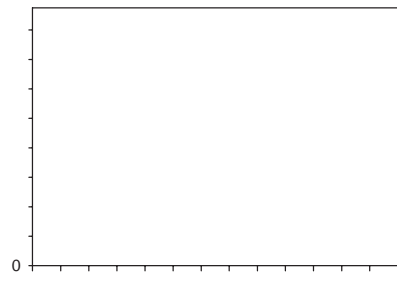
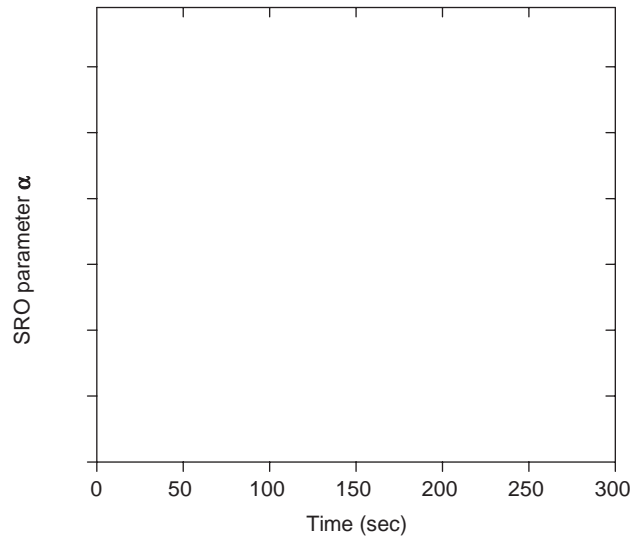


Fig. 5. The number of precipitates N versus time t [sec] for different temperatures $T = 200, 250, 300$ K. The solid lines represent the simulation results, and the dashed line represents the theoretical prediction with a slope of -1 .

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





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