

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

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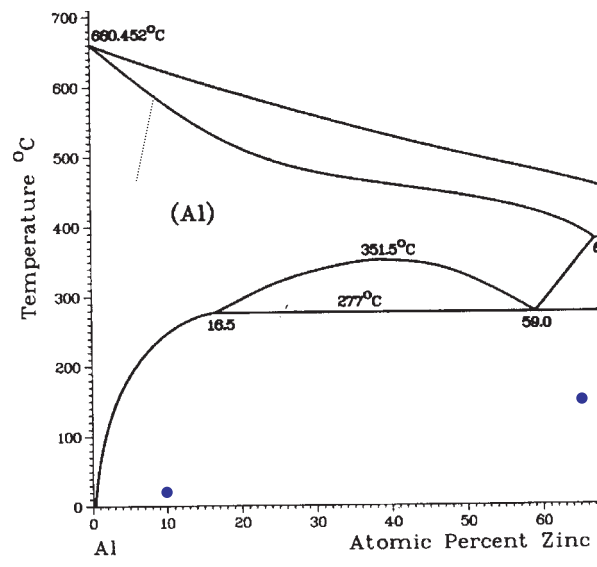
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\mathbb{W} is the set of all possible configurations of the system. The energy of a configuration \mathbf{W} is given by $E(\mathbf{W})$. The partition function Z is defined as $Z = \sum_{\mathbf{W}} e^{-\beta E(\mathbf{W})}$, where $\beta = 1/(k_B T)$. The average energy $\langle E \rangle$ is given by $\langle E \rangle = -\partial \ln Z / \partial \beta$. The entropy S is given by $S = -k_B \sum_{\mathbf{W}} p(\mathbf{W}) \ln p(\mathbf{W})$, where $p(\mathbf{W}) = e^{-\beta E(\mathbf{W})} / Z$. The free energy F is given by $F = \langle E \rangle - TS$.

2. t

2.1. Cluster expansion of substitutional configurational energies

The total energy $E(\sigma)$ of a configuration σ can be expanded in terms of cluster functions $J_n(\mathbf{k}, \sigma)$ as follows:

$$E(\sigma) = \sum_{\mathbf{k}} J_1(\mathbf{k}, \sigma) + \frac{1}{2} \sum_{\mathbf{k}} J_2(\mathbf{k}, \sigma) + \frac{1}{6} \sum_{\mathbf{k}} J_3(\mathbf{k}, \sigma) + \dots$$

where \mathbf{k} is a cluster of sites. The cluster functions $J_n(\mathbf{k}, \sigma)$ are defined as the energy of a cluster \mathbf{k} minus the energy of the same cluster in the reference state. The reference state is usually taken to be the state where all sites are occupied by the most abundant species.

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

The cluster functions $J_n(\mathbf{k}, \sigma)$ can be further expanded in terms of pair functions $J_{ij}(\mathbf{k}, \sigma)$ as follows:

$$J_n(\mathbf{k}, \sigma) = \sum_{i,j \in \mathbf{k}} J_{ij}(\mathbf{k}, \sigma) + \dots$$

where $J_{ij}(\mathbf{k}, \sigma)$ is the energy of a pair of sites i and j in the cluster \mathbf{k} . The pair functions $J_{ij}(\mathbf{k}, \sigma)$ are defined as the energy of a pair of sites i and j in the cluster \mathbf{k} minus the energy of the same pair of sites in the reference state. The pair functions $J_{ij}(\mathbf{k}, \sigma)$ can be further expanded in terms of single-site functions $J_i(\mathbf{k}, \sigma)$ as follows:

$$J_{ij}(\mathbf{k}, \sigma) = J_i(\mathbf{k}, \sigma) + J_j(\mathbf{k}, \sigma) + \dots$$

where $J_i(\mathbf{k}, \sigma)$ is the energy of a single site i in the cluster \mathbf{k} . The single-site functions $J_i(\mathbf{k}, \sigma)$ are defined as the energy of a single site i in the cluster \mathbf{k} minus the energy of the same single site in the reference state.

... (1). (2) ... $D_{\text{eff}}(\omega)$... $1/\tau_0$... $D_{\text{eff}}(\omega)$...

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

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 $-1 + 1/$ ($1, \dots, N$)
- $\delta E(i)$.
- 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} $\delta E(i)$ *no longer a constant real time unit*, $1/1000$.

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

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

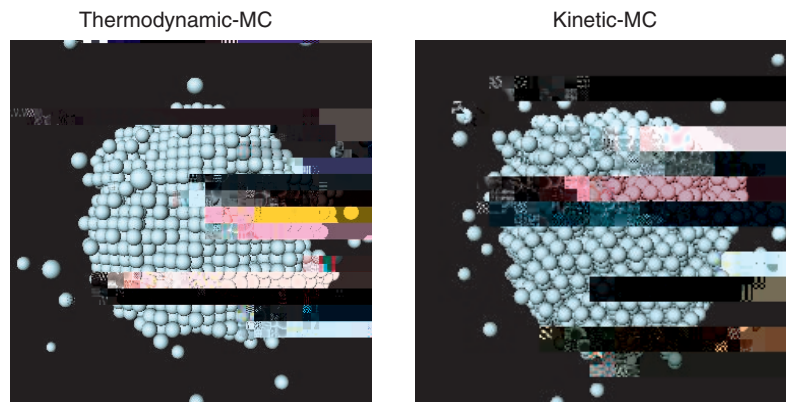
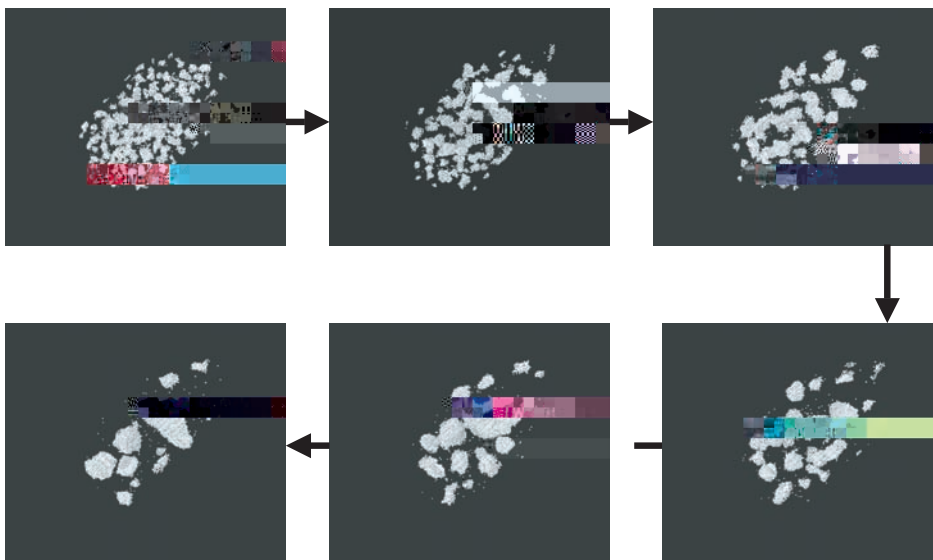


Figure 2. Molecular dynamics simulation of protein-ligand complex using Thermodynamic-MC (left) and Kinetic-MC (right) for 100 ns. The protein is shown as a grey surface, and the ligand is shown as a stick model with various atoms colored (red, yellow, blue, green).

Table 1. Molecular dynamics simulation results for protein-ligand complex using Thermodynamic-MC and Kinetic-MC.

Table 4: α values for the $(0, 1)$ distribution. The values are calculated using the $(0, 1)$ distribution with $\alpha = 0.2$ and $\alpha = 0.0$. The values are calculated using the $(0, 1)$ distribution with $\alpha = 0.2$ and $\alpha = 0.0$.

()	$\alpha = 0.2$	$\alpha = 0.0$
000	1.000	1.000
110	0.400	0.000
200	0.400	0.200
211	0.100	0.010
220	0.300	0.300
10	0.300	0.300
222	0.300	0.100
21	0.200	0.110
400	0.100	0.000
0	0.300	0.300
411	0.020	0.000



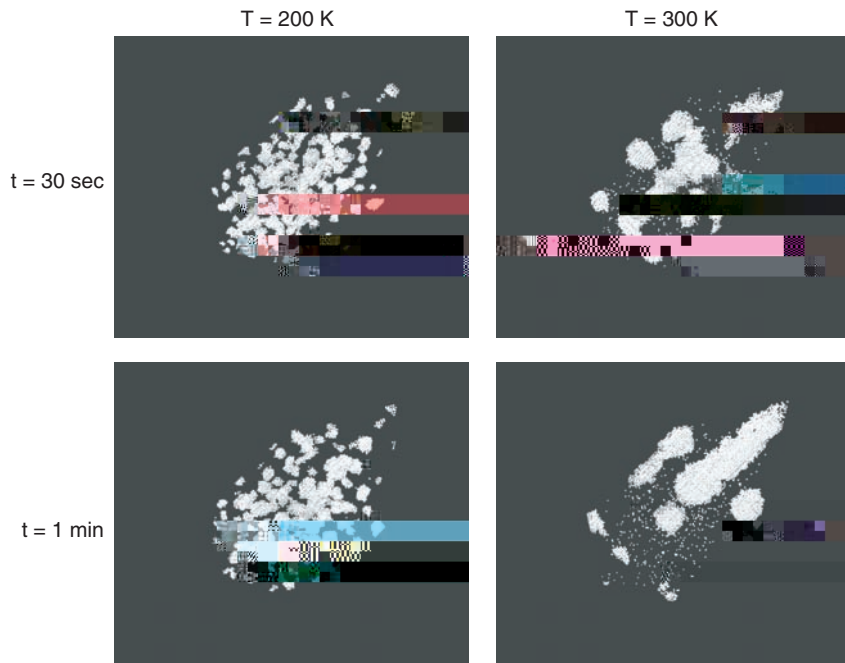


Fig. 4. Morphology of precipitates at different temperatures and times. The precipitates are shown in white, and the surrounding matrix is shown in black. The colors in the matrix represent different phases.

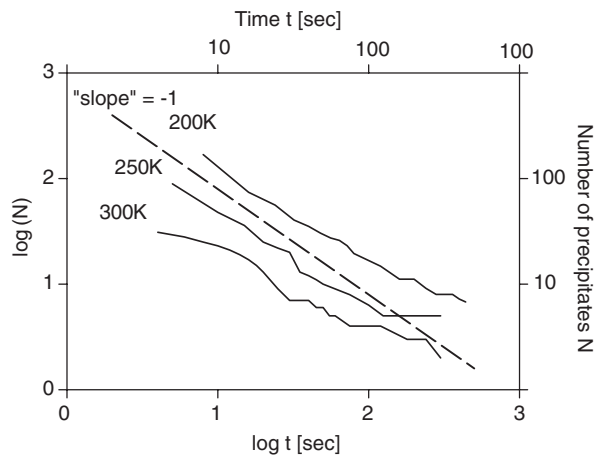
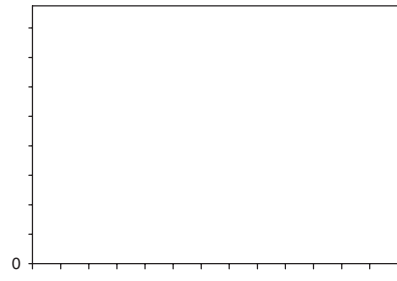
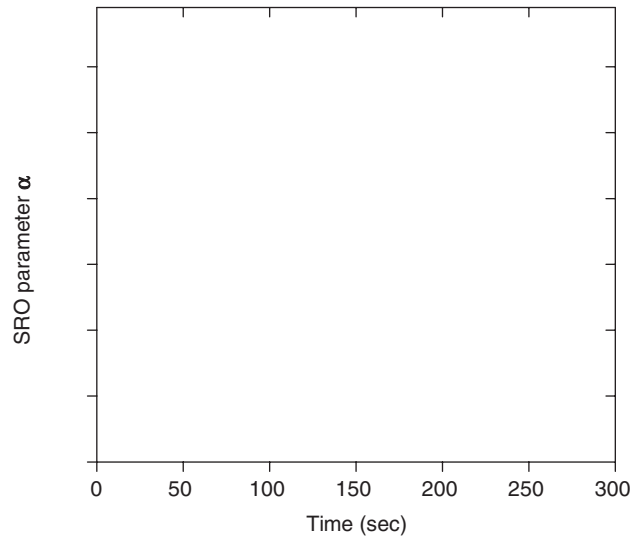


Fig. 5. Log-log plot of the number of precipitates N versus time t for different temperatures. The solid lines represent the experimental data, and the dashed line represents the theoretical prediction with a slope of -1.

The number of precipitates N decreases over time for all temperatures. The rate of decrease is more pronounced at higher temperatures. The theoretical prediction with a slope of -1 is shown for comparison.





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