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

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the size distribution compared with higher agency temperatures. (iii) After the initial formation  $\epsilon$ of precipitates within the first few seconds for a given temperature and concentration, the shortrange order parameters order parameters of the allowing only show a weak time dependence. In the following, we ه و توسط الرسم الأمر من اللغاء بي المدام التي تعرف بحالته التي تركو من في الحكم وكان العام التي الرسم على المد<br>و تتعلق الرسم الأمر من اللغاء بي المدام التي تعرف بحالته التي تركو من في الحكم العام التي التي تتوسط العام الم  $f_{\rm obs}$  , principles  $L$  based cluster expansion  $21$  . Using our theoretical model, we will study, we will study, as a function of agent of agent of  $G$  clusters at distribution of  $\chi$  clusters at different temperatures, (ii number of precipitation of time evolution of the short-range order range order order order order order order o will compare our results with those expected from classical Ostwald ripening which would predict a <sup>1</sup>/ evolution for the average precipitate diameter.

## **2.** t

## *2.1. Cluster expansion of substitutional configurational energies*

 $\mathcal{T}_{\text{c}}$  energy  $E_{\text{c}}(\sigma)$  of substitutions is given by a mixed-space cluster expansion by a mixed-space configurations is given by  $(\Box)$  [21]. In this approach, any configuration  $\sigma$  is defined by specifying the occupations of each of the N  $_l$  atom (spin index  $_l$  and  $_l$  atom (spin index  $-1)$  or a Zn atom (  $-$  +1). The formation enthalpy of any substitutional configuration σ at its atomically relaxed state is then  $\mathcal{T}_{\infty}$  given by

$$
\Delta H \quad (\sigma) \qquad \sum_{k} J_{\dots} (k) \quad (k, \sigma)^2 + \sum_{k} D \quad J \quad \Pi \quad (\sigma) + \frac{1}{4} \sum_{k} \Delta E \quad (\quad , \quad) \quad (k, \sigma)^2. \tag{1}
$$

The first sum describes all possible pair figures. It is expressed in reciprocal space, thus affording a converged description of even long-range pair interactions [28]. Here, Jpair(*k*) is the lattice Fourier transform of the real-space pair interactions, and S(*k*,σ) are structure factors. The second sum describes many-body (MB) figures, such as triangles, tetrahedra, etc. Here,  $J$  is the real-space many-body interaction of figure ,  $D$  stands for the number of the number of equivalent clusters per lattice site, and  $\Pi$  ( $\sigma$ ) are spin products. The last term in equation (1)  $(1)$ describes the constituent strain energy necessary to maintain energy necessary to maintain coherence  $\Lambda$ fcc Zn along an interface with orientation . It can be calculated by deforming the bulk elements the bulk elem  $(\lambda_{\rm crit})$  for  $\lambda_{\rm crit}$  from the from their equilibrium lattice constants  $\lambda_{\rm crit}$ perpendicular to . We see that the first two terms in equation (1) describe *atomistically* the 'chemical energy' of a configuration, which term describes the third term describes the anisotropic (and  $\alpha$  $g_{\rm max}$ long-range strain energies. Long-range strain energies. Long-range strain energies. Long-range strain energies. Lo

 $U''$  determine  $J_{\mu\nu}(k)$  and  $J_{\mu\nu}$ 

spin-flips always correspond to geometrically fully relaxed configurations. This is guaranteed configurations o by our MSCE-Hamiltonian of equation (1). (ii) Our model does not have vacancies. (iii) In order to consider the energy barriers between different configurations, we accept informations, we ac from experiment: of jump frequencies,  $1/\tau_0,$  as a function of temperature were taken from the taken from the experimental diffusion constant  $D_{\rm eff}(\mathbb{C})$  via

$$
\tau_0(\ )\qquad \frac{2}{|D_{\cdot}|(\ )},\tag{2}
$$

where  $\mathcal{E}(\mathbf{z})$ 

forbid this second step in the simulation, we would be confronted with a non-Markovian process demanding a complex reconsideration of the function between experimental diffusion حردي المداوية والمستخدمة السراكية المتوادع بالمواقع التجارية المستخدمة التي يتوجه في السراران المواطنة والمستخدمة المرتكز بن الموارد والمركز التاريخية والمركز التاريخ والمركز الموارد المركز والمركز الموارد والمركز الموارد والمر<br>المركز الموارد المركز الموارد المركز الموارد والمركز الموارد الموارد المركز الموارد الموارد الموارد الموارد certain Zn atom to jump back to the precipitate surface in MCS number , from which it was number , from which i removed in MCS number −1, it is very likely that this 'returning' event will happen in MCS number  $+1.$  The best solution for the the above problem seems to be an algorithm where the an algorithm where the the theorem  $\alpha$ chosen  $\mathcal{L}_{\text{c}}$  atom is  $\mathcal{L}_{\text{c}}$  without destroying the Markovian process. This is realized in the following algorithm—algorithm II:

- $1.$  Find all of the N  $\le$  atoms in a random configuration and order them by site indices. The model them by site indices. 2. Determine all the possible jumps for  $\epsilon$  and  $\epsilon$  and  $N$  at  $\epsilon$  lattice  $\epsilon$  at  $\epsilon$ max  $12N_{\rm gas}^{\rm H}$  and  $\alpha_{\rm m}$  are atoms as neighbours). The  $\alpha_{\rm m}$  $3.$  Calculate the energy change  $\delta E(.)$  for  $each$  all  $i$  for all  $\epsilon$  and  $i$  atoms (  $1,\ldots,$  ).
- $4. \int_{1}^{1} \delta E(t) > 0,$   $4. \int_{1}^{1}$ .  $4. \int_{1}^{1} (1/\tau_{0}) e^{-\int_{0}^{t} (-\delta E(t))} \int_{1}^{t} \delta E(t) < 0,$   $4. \int_{1}^{1} e^{-\delta E(t)}$ 4  $\cdot$   $\int_0^{\pi} \frac{\delta E(t)}{\delta t}$  > 0,  $\cdot$   $\int_0^{\pi}$
- $\mathcal{F}_1$  .  $\mathcal{F}_2$  /with  $\mathcal{F}_3$  and  $\mathcal{F}_4$  .  $\mathcal{S}(\epsilon)$  select randomly one jump from the possible events according to the probability  $P$  . 7. Calculate the new total simulation time MCS−1 + 1/Wtot. (Note that  $\sum$ tot player and start player and the start of t  $\frac{1}{1}$  is a notation for each method  $\frac{1}{1}$  is different for each  $\frac{1}{1}$  , and  $\frac{1}{1}$  after each  $\frac{1}{1}$  $\label{eq:3} \mathcal{L}=\left\{ \left\vert \mathcal{L}_{\mathcal{M}}\right\vert ^{2},\left\vert \mathcal{L}_{\mathcal{M}}\right\vert ^{2}\right\}$  $\mathcal{E}(\cdot)$   $\mathcal{E}(\cdot)$ 's.
- 9. Go back to step 4.

 $\mathcal{T}_{\phi}$  efficiency of this method strongly depends on the calculation of whether the calculation of  $\phi$ the new  $\delta E(\cdot)$ 's (step 8) is time international and accepted spin-flip demonstration of plane as  $\delta$  $S_k(\mathbf{k},\sigma)$  in equation (1). However, as shown by Lu  $e$  allows one to  $\mathbf{k}$  $\alpha$  and the necessity of recall  $(k, \sigma)$  at  $\alpha$  and  $\alpha$  after each move by directly calculation  $\sigma$  $\int_{\mathbb{R}^n}$   $\int_{\mathbb{R}^n}$  (k,  $\sigma$ ) 2 for each move in real space  $\int_{\mathbb{R}^n}$  is considered in product  $\int_{\mathbb{R}^n}$ for short ageing times and high temperatures, i.e. where nearly every flip is accepted. The advantage of algorithm II lies in the simulation of long agents times. As we can see from  $\alpha$ step 4 of the algorithm description, now a single MCS is *no longer a constant real time unit*, but depends on the corresponding probability tot. In practice, one MCS can now represent real times  $1/1000$  s up to many minutes. As a rough  $\epsilon$  real conclude that algorithm III  $\epsilon$  algorithm III is to be preferred, if one MCS corresponds to a real time of about 1 s.

It should be mentioned that in algorithm II and indeed that in algorithm II a single MCS corresponds in the  $\int_{\mathbb{R}^d} \left| \frac{1}{\sqrt{n}} \right| \, d\mu$ flip of one Zn atom and *not* one trial-flip of each Zn atom. Since flip channel is always chosen randomly and we most large number of Zn atoms (e.g. 1000–1500 $($  g.  $(0.5, 1000)$   $(1, 000)$  , the probability that the same Zn atom is chosen in MCS , when it was already chosen in MCS  $-1,$  is very small. So, due to the large system system size, it is not necessary to forbid any kind of  $\alpha$ jumps between  $\mathcal{A}_1$  and  $\mathcal{A}_2$  and  $\mathcal{A}_3$  atoms, i.e. we do not have to give up that the algorithm that the algorith showled be based on the Markovian process. The conceptibility is very similar to that  $\mathcal{E}_t$ of the so-called the so-called transition  $\pm 11$  , where  $\pm 1$  and the so-called at each  $\pm 1$  at each  $\pm 1$ MCS. Different from the work of Soisson *et al* [33], who applied such an algorithm to study Cu precipitation in Fe–Cu alloys, our model does not consider any vacancy jump mechanism. ما يأت والدينيات التأميني بالمن والمعاطي المحافظة والمتحدث والتأمين المنافس المنافس المنافس المنافس المنافس ال Our present kinetic simulations are restricted to neare restricted to nearest-neighbour  $\mathbb{U}_{\mathrm{in}}$  is not in generally justified, although it was already successfully applied in the literature (see e.g.  $(18)$ ). For certain applications, a necessary extension to second, the certain to second, the model of third, and the s may be needed.



 $F: \mathbf{F}^{2}$ . Comparison between explicit  $\mathcal{A}_{\text{max}}$  and  $\mathcal{A}_{\text{max}}$  allow  $\mathcal{A}_{\text{max}}$  resulting from  $\mathcal{A}_{\text{max}}$ thermodynamic and kinetic MC simulations (only Zn atoms are shown).

Both algorithms fulfil the condition of detailed balance. Although the kinetic MC  $\sim$ 







**Figure 4.** Zn precipitates in Al–Zn for two different ageing temperatures and times. For a constant الجاذب الموطنات التي والمحاكم والاستعمالي والتجارية الموجود الجادل المداري والمحاصر التي تعالي المدار الموارد والمستخدمات المدار  $\ldots$  ).



**Figure 5.** Logarithmic plot of number of precipitates versus ageing time in an Al0.932Zn0.<sup>068</sup> alloy (11.4.  $2$  ) atoms) for the slope of atoms of all three curves is very close to all three curves is very close to  $\mathcal{I}_\text{c}$ −1, i.e. the expected value for classical operation (- - -).

. الأسهى ومن المعادات الرادد العالم والمقاط والمتماثلين مدارات ومعهد المتخلصة بالمحاد المتألف المتوسط في العنادات ومتهادم والم system size. So, e.g. for an agent temperature of  $2/0$  K and an agent and an agent time of  $\zeta$  min, there are are are are assumed to  $\zeta$ وهم به دار برای داد در ادامه آن این سری ایجاده 11 و دانشمنده به دام به استاد به سام 1 مربوط با در دانشمند به استاد است. m, of all precipitation of all precipitation of agency of agency  $\ell$  , m represents the sentent of a function of a diameter of the corresponding sphere having the same volume as the observed precipitate.





 $\mathcal{F}$  . Distribution of precipitation of precipitation  $\mathcal{F}_{\mathcal{F}_1}$  and  $\mathcal{F}_2$  (  $\mathcal{S}_3$  ).

**4. t t**  $t$  **f**  $t$  $\pi$  short-range order (SRO) can be described in terms of the Warren–Cowley SRO parameters of the Warren which are given for shell  $(\mathcal{L})$ 

$$
\alpha \quad (\quad) \quad 1 - \frac{P^{A(B)}}{\cdot}, \tag{}
$$

where  $P^{A(B)}$  is the conditional probability that, given an  $A$  atom at the origin, the origin, the origin, the  $B$  atom at (lmn). The sign of  $\alpha$  indicates shell preference shell preference shell preferences in a given shell  $\alpha > 0$  order ( $\alpha < 0$ ),  $\alpha > 0$ . The SRC parameter may be written in terms of the pair correlations as a correlation of the correlation of the correlation of the correlations of the correla

$$
\alpha \quad (\quad ) \quad \frac{\Pi \quad -\quad ^2}{1-\quad ^2}, \qquad \qquad (4)
$$

where  $2 - 1$  and lmn is the pair correlation function function  $\frac{1}{\ln(1-\delta)}$  . In different والتعالي المستعمر المواسم ومن المستعمر المرحم المرتبي المستعمر الكرام المعاصر من المستعمر المستعمر المتمول الم  $t$  transform of  $\alpha$  almost  $\alpha$  (iii):

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



[13] Wang Y, Chen L-Q and Khachaturyan A G 1991 *Scripta Metall.*