



# A thermo-kinetic correlation for grain growth in nanocrystalline alloys

H.R. Peng, L.K. Huang, F. Liu\*

State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, 710072 Xi'an, PR China



## ARTICLE INFO

### Article history:

Received 18 January 2018

Accepted 24 February 2018

Available online 24 February 2018

### Keywords:

Activation energy  
Grain boundary energy  
Segregation  
Correlation

## ABSTRACT

The thermo-kinetic stabilization that incorporates mixed effects of grain boundary (GB) energy and activation energy for GB migration has shown enormous advantages in describing thermal stability of nanocrystalline materials. However, its underlying physics is still unclear due to the lack of proofs that the two effects coexist and act together to impact on grain growth. In this work, a thermo-kinetic correlation is derived to bridge GB energy and activation energy in nanocrystalline alloys. Meanwhile, molecular dynamic simulations are performed to determine the two parameters in Al-based systems. The results shows that upon GB segregation, the GB energy is reduced in contrast with the increased activation energy. This analytically suggests a thermo-kinetic origin for stabilization due to GB segregation, other than pure thermodynamic or kinetic sources.

© 2018 Elsevier B.V. All rights reserved.

## 1. Introduction

Nanocrystalline (NC) materials exhibit uniquely mechanical and engineering properties that are often superior to their coarse-grained counterparts [1]. However, due to the high-density grain boundaries (GBs), these materials generally lack microstructural stability with increasing temperature that limits their engineering applications [2]. Therefore, stabilizing grain sizes of NC materials has been becoming a quite important topic in the field of nano-processing and application.

Alloying foreign atoms into the matrix has been demonstrated as one of the most effective ways to stabilize grain sizes of NC materials; two approaches/mechanisms must be mentioned: one is thermodynamic stabilization achieved by reduced GB energy [3,4] and the other is kinetic stabilization arising from increased activation energy [5,6]. Since the thermodynamic approach pays attention to equilibrium or meta-equilibrium state whereas the kinetic approach points to grain growth process, the two stabilization approaches are generally considered as non-coexistent and independent of each other in past studies. This, however, leads to fundamentally different interpretations for stabilization in, e.g. Ni-W system, where Choi et al. attributed grain growth inhibition to low mobility of W atoms [7] while Trelewicz and Schuh accounted for stability by reduced GB energy [8]. Such controversial interpretations for the stabilization can also be found in Pd-Zr system [2]. A thermo-kinetic stabilization, where the thermodynamic and the kinetic stabilizations coexist and act together

to impact on grain growth, was then proposed [9,10]. After that, great successes have been achieved in understanding the thermal stability of NC alloys. However, two inherent flaws must be highlighted: the framework of thermo-kinetic stabilization is based on either the arbitrary incorporation of the expressions of GB energy and solute drag [9] or the roughly semi-empirical equation [10]; the functional relation describing the interaction between the thermodynamics and the kinetics, i.e. the thermo-kinetic correlation, is still unavailable. This kind of correlation, if confirmed, depicts a fundamental law governing the thermodynamics and kinetics of GB migration in NC alloys.

Here we derive a thermo-kinetic correlation that addresses how the thermodynamics is analytically related to the kinetics in NC alloys, through characteristic parameters of solute/solvent atoms. Furthermore, we prove it by molecular dynamic (MD) simulations in Al-Ni and Al-Sm systems.

## 2. Model derivations

We focus on NC alloys without precipitation of solute-rich phases and the GB migration is kinetically inhibited by the solute drag effect, which leads to an increase of activation energy for GB migration ( $Q$ ). Previously, since the function relation between  $Q$  and GB excess ( $T_A$ ) is unavailable,  $Q$  is roughly assumed as a constant independent of grain growth, which cannot reflect the physics of kinetic process. Aiming to obtain a  $T_A$ -dependent  $Q$ , it is inevitable to reanalyze the solute drag effect. Following Cahn's model [6], the solute drag effect only depends on the segregated solute atoms with the GB excess as  $T_A = \Gamma_A/A_m^{GB}$ , where  $A_m^{GB}$  is the molar GB area and  $\Gamma_A$  the difference between solute

\* Corresponding author.

E-mail address: [liufeng@nwpu.edu.cn](mailto:liufeng@nwpu.edu.cn) (F. Liu).

concentrations in GBs and bulk. If dividing all the atoms in GBs into two parts, i.e. the segregated solute atoms (with the amount as  $\Gamma_A$ ) and the remaining atoms (with the amount as  $1 - \Gamma_A$ ), only the former should contribute to the increase of  $Q$ . Following Rawlings et al.'s model [11], the segregated solute atoms should overcome an energy barrier  $Q^b + H_{seg}$  (with  $Q^b$  as the activation energy of bulk diffusion and  $H_{seg}$  the segregation enthalpy) to move forward to the GBs. Assuming the intrinsic activation energy as  $Q_0$ , the overall contributions from the two parts of atoms give the expression of  $Q$

$$Q = (1 - \Gamma_A)Q_0 + \Gamma_A(Q^b + H_{seg}) = Q_0 + \Gamma_A(H_{seg} + \Delta Q) \quad (1)$$

where  $\Delta Q = Q^b - Q_0$ . Clearly, Eq. (1) reflects the increased kinetic stabilization effect exerted by the segregated solute atoms. Meanwhile, the segregated solute atoms generally reduces the GB energy; this physics can be described by the GB energy model from Krill et al. [4]

$$\gamma = \gamma_0 - \Gamma_A \frac{H_{seg}}{A_m^{GB}} \quad (2)$$

where  $\gamma_0$  is the GB energy of pure solvent and the entropic contribution is ignored. Combining Eqs. (1) and (2) gives

$$\frac{Q - Q_0}{\gamma_0 - \gamma} = \frac{H_{seg} + \Delta Q}{H_{seg}} A_m^{GB} \quad (3)$$

Eq. (3) indicates a thermo-kinetic correlation, i.e.,  $\gamma$  is reduced in contrast with increased  $Q$ .

### 3. Simulation methods

As shown in Fig. 1(a), a bicrystal model containing two identical GBs is constructed. The  $\Sigma 5$  symmetric tilt GB in Al-based alloys is used, whose atomic configurations is shown in Fig. 1(b). Various

numbers of Ni/Sm atoms are introduced into GBs to randomly replace the Al atoms there (see Fig. 1(c)). Using embedded-atom method potentials for Al-Ni [12] and Al-Sm [13], the present simulations are performed at 825 K with the boundary identified by the non-fcc coordinated atoms. The synthetic driving force is added in the grain 1 so that the two GBs would move towards each other, where the thermal fluctuation of GBs can be described by [14]

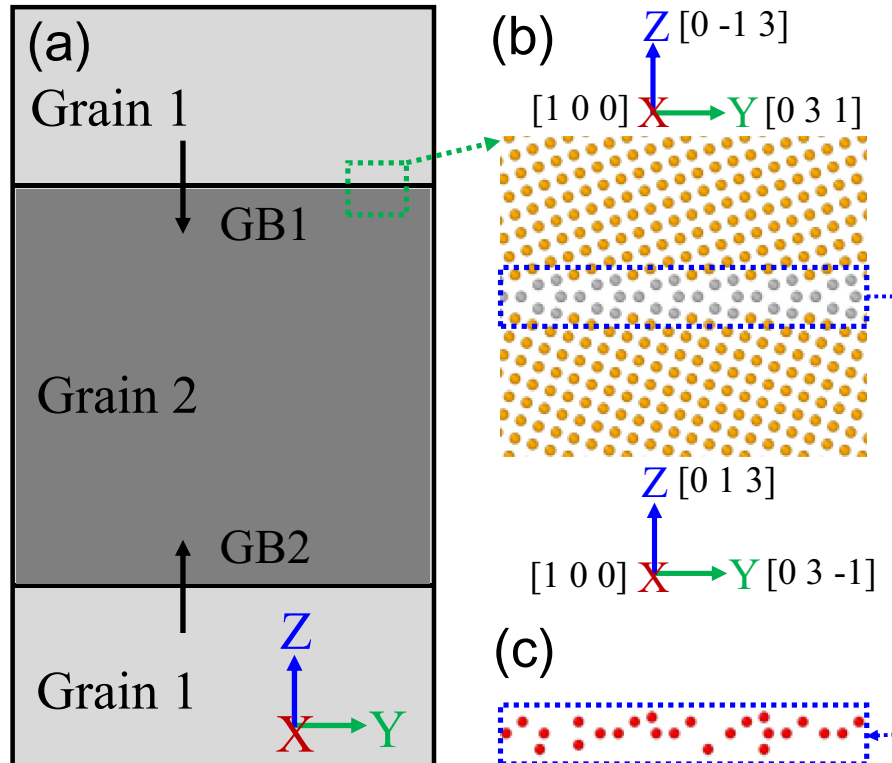
$$D^{GB} = \frac{d \langle d^2 \rangle}{dt} = \frac{2MkT}{A^{GB}} \quad (4)$$

with  $D^{GB}$ ,  $t$ ,  $\langle d^2 \rangle$ ,  $T$  and  $A^{GB}$  as the diffusion coefficient, the time, the mean square displacement (MSD), the temperature and the GB area, respectively.  $M$  is the GB mobility, which follows an Arrhenius equation with  $Q$ , i.e.  $M = M_0 \exp(-Q/RT)$ . Inserting Eq. (1) into the expression of  $M$  and applying a logarithmic transformation lead to

$$\ln M = -\frac{Q}{RT} + \ln M_0 = -\Gamma_A \frac{H_{seg} + \Delta Q}{RT} + \ln M_0 - \frac{Q_0}{RT} \quad (5)$$

### 4. Results and discussions

As shown in Fig. 1(c), solute atoms are initially located in GBs. With prolonging the simulation, the evolution of solute position and GB position almost overlap with each other in both Al-Ni and Al-Sm, suggesting solute segregation in GBs [15]. Furthermore, following the statistical methods in Ref. 14, the MSD is calculated, whose evolution with time is shown for various number of Ni and Sm atoms in Fig. 2(a) and (b), respectively. On this basis, GB mobility is extracted according to Eq. (4) and shown in Fig. 2(c); clearly,  $\ln M$  decreases approximately linearly with the number of solute atoms. Assuming  $M_0$  as a constant independent of the temperature and performing MD simulations at 800, 825 and 850 K,  $M_0$  is



**Fig. 1.** (a) Schematic of the bicrystal model with synthetic driving force applied to the GBs. (b) The relaxed atomistic configuration of the  $\Sigma 5(3\ 1\ 0)$  symmetric tilt GBs of Al. (c) Random distribution of solute atoms in GBs of Al.

Download English Version:

<https://daneshyari.com/en/article/8013884>

Download Persian Version:

<https://daneshyari.com/article/8013884>

[Daneshyari.com](https://daneshyari.com)