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# The effects of lattice misfit on grain boundary phase transformation

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## 1.Research background

Precipitation strengthening is the most effective approach to improve the mechanical properties of aluminum alloys[1]. The optimization and precise control about the structure, distribution, shape, size, and fraction of precipitates are crucial considerations in developing and fabricating advanced aluminum alloys. Generally, precipitation may occur in both grains' interior and grain boundaries (GBs) of polycrystalline alloys. Compared with the interior of grains, GBs are relative loose and disordered, and thus solute atoms tend to be enriched in GBs, facilitating the precipitation in GBs consequently[2]. Moreover, as the weakness of polycrystalline materials, GBs determine the mechanical properties of the whole material. Previous studies reported that GB precipitation could greatly change the microstructure of GB, such as the formation of precipitation free zone and phase boundaries, the variations in intergranular structure, and so on, and consequently probably brings significant effects on the strength, plasticity and corrosion resistance of GBs, and the performance of polycrystalline materials ultimately.

The purposes of the present work

1. 1. The clustering around dislocation and grain boundaries are successfully simulated on atomic scale through phase-field crystal model. The influence of these structures on clustering are investigated.
2. The result show that symmetrical grain boundaries tend to give rise to polycrystalline clusters. Double-nucleus also appear firstly on asymmetric grain boundaries, however only nucleus remains.
3. Different cluster behavior at low angle grain boundaries and high angle grain boundaries indicates that nucleation is more likely to occur at large angle boundaries.

## 2. Simplified binary free-energy functional

The free energy for a binary PFC model can be written as a combination of the energy of the two density fields separately and a component including their interaction. The total free energy is written form as

$$F=\int dr\{\frac{n^2}{2}-\nu\frac{n^3}{6}+\xi\frac{n^4}{12}+\omega\Delta F_{mix}(n+1)-\frac{1}{2}n\int dr' C_{eff}(|r-r'|)n(r')+\frac{\alpha}{2}|\nabla c|^2\}$$

The entropy of mixing is modified according to

$$\Delta F_{mix}=c\ln\frac{c}{c^0}+(1-c)\ln\frac{(1-c)}{(1-c_0)}$$

The effective correlation function in the free energy is a polynomial ,weighted by the composition field.

$$C_{eff}=X_1(c)C_2^{AA}+X_2(c)C_2^{BB}$$

The dynamics of the total density and concentration fields obey the usual dissipative dynamics applied to each species density, this translates to the following equations of motion for n and c:

$$\frac{\partial n}{\partial t}=\nabla\cdot M_n\nabla\{n-\nu\frac{n^2}{2}+\xi\frac{n^3}{3}+\omega\Delta F_{mix}-\int dr' C_{eff}(|r-r'|)n(r')\}$$

$$\frac{\partial c}{\partial t}=\nabla\cdot M_c\nabla\{\omega(n+1)\frac{\partial\Delta F_{mix}}{\partial c}-\frac{1}{2}n\int dr'\frac{\partial C_{eff}(|r-r'|)n(r')}{\partial c}-\alpha\nabla^2 c\}$$

## 3. Eutectic phase diagram construction and simulations of clustering

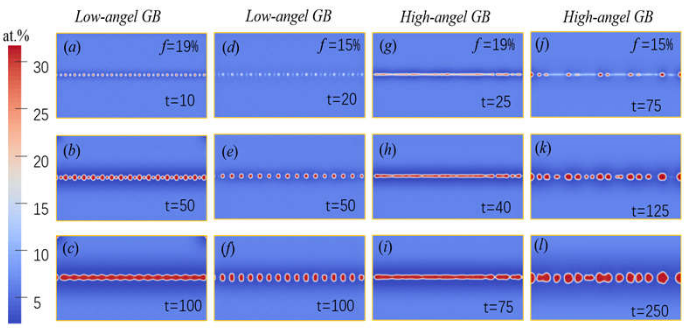


Fig.1 The evolution of GB precipitation distribution with GB structure and lattice misfit. (a) Low-angle GB with lattice misfit 19%; (b) low-angle GB with lattice misfit 15%; (c) high-angle GB with lattice misfit 19%; (d) high-angle GB with lattice misfit 15%.

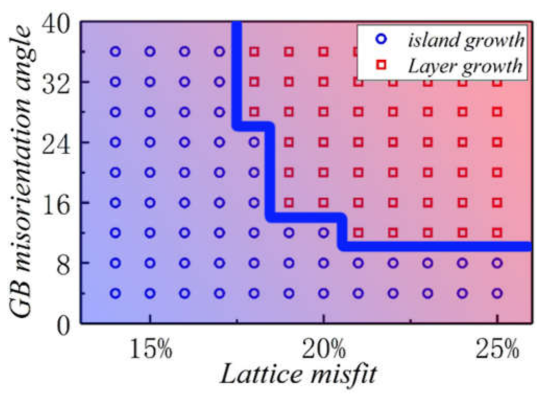


Fig.2. The sketch about the selection of growth modes of GB clusters with respective to GB structure and lattice misfit.

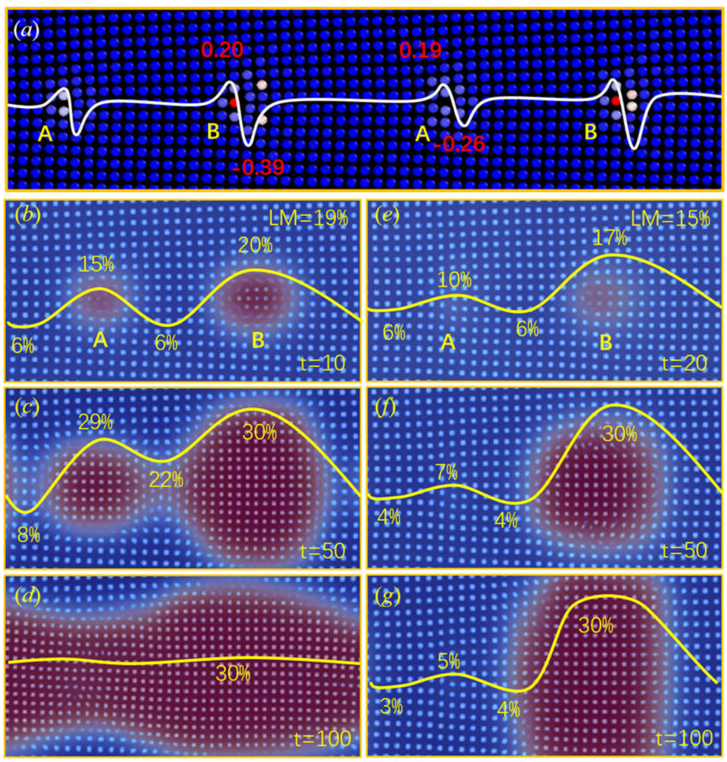


Fig.3 (a)The microstructure of low-angle GBs. The white curve represents the strain around the GB. The influence of lattice misfit on lattice orientation on low-angle GBs. Low-angle GB with lattice misfit 19%. (b) t=10, (c) t=50, (d) t=100. Low-angle GB with lattice misfit 15%: (e)t=20, (f) t=50, (g) t=100. The yellow curves represent the concentration of solute around the GB.

## 4. Conclusion

- GB precipitation tends to island growth in alloy with low lattice misfit, while tends to layer growth in alloy with high lattice misfit. Besides, the high-angle GB is conducive to layer growth, and the low-angle GB is conducive to island growth.
- For some regions that are difficult to nucleate, increasing the lattice misfit can reduce the potential barrier of nucleation and promote the process of nucleation.

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Reference:

[1] P. Rambabu, N. E. Prasad, V. V. Kutumbarao, and R. J. H. Wanhill, Aluminium Alloys for Aerospace Applications 2017).

[2] B. Milkereit, M. Reich, and O. Kessler, Materials Science Forum 877, 147-52 (2017).