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Mechanisms of θ′ precipitation in Al-Cu: strain energy role in heterogeneous nucleation and ledge growth

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1 Introduction

Coherent precipitation in solid matrix is strongly influenced by the matrix-product transformation strain. Although experimental evidence suggest significant shear component in the formation of θ′ precipitates, this fact is largely ignored in the nucleation and microstructure development models available in the literature. Thus existing mesoscopic models fail to explain adequately the morphology, growth kinetics and autocatalysis in Al-Cu precipitation hardening.

Here we attempt to look at the existing transformation mechanisms which recognize the lattice correspondence with large shear component. The influence of shear on homogeneous nucleation is studied. Heterogeneous nucleation of θ′ on static defects and in autocatalytic mode is discussed.

2 Transformation mechanisms

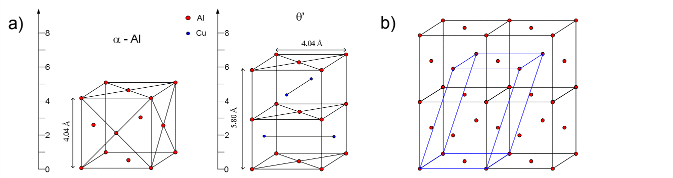
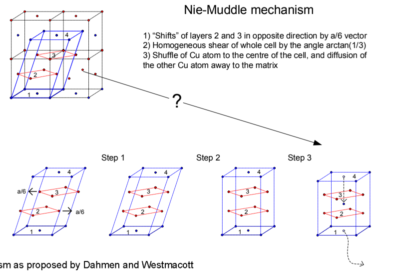
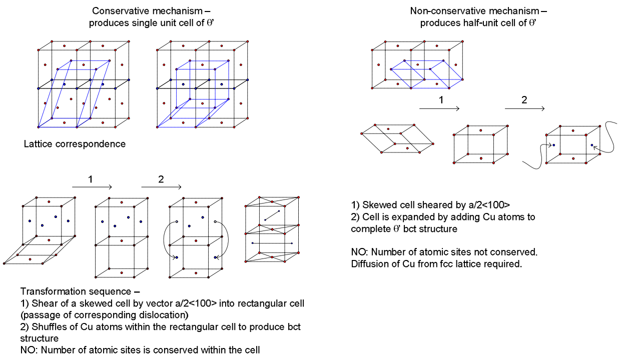


Fig 1 Structure of fcc Al-matrix and bct θ′; Lattice correspondence for fcc Al-Cu to θ′ transformation

Transformation mechanism with lattice correspondence in Fig.1,b was proposed by Dahmen and Westmacott [1], and similar lattice correspondence was employed by Nie and Muddle [2]. Main feature of these mechanisms is a significant shear component equal to 0.33, accompanied by the contraction in c-direction





3 Growth with shear accommodation

Experimentally observed thickness of plates [3] is well explained in frame of transformation mechanism proposed by Dahmen and Westmacott (illustrated above). Two mechanisms are combined to minimize both shape (by self-accommodation of the shear component) and volume (by mixing blocks with contraction and expansion) change during growth of the plate. Thus two elementary "building" blocks are:

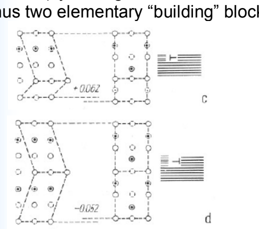


Fig 2 Self-accommodated building blocks [1]

Hence minimal possible thickness for θ′ plates is 2 unit cells, followed by 3.5 (formed with type **c** ledge), then 5.5, 7 etc.

Experiment [3] confirms the sequence except for the number of observed particles 5 unit cell thick.

Moreover, one unit cell thick plates of θ′ are invariably associated with a/2<100> dislocations accommodating shear part of the transformation.

References

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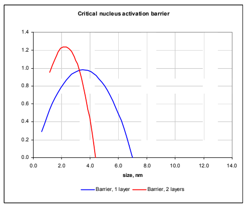
4 Homogeneous nucleation

Activation energy required for homogeneous formation of the nucleus could be estimated in frame of the classical nucleation theory. Analytical solution for the elastic energy of the coherent ellipsoidal inclusion [4] allows to fully relax nucleus configuration in size-shape space, and compare parameters of self-accommodated (with respect to shear) vs non-accommodated nucleus.

Table 1. Critical nucleus parameters at different driving forces for purely tetragonal distortion of 4.3% (top rows) vs tetragonal+shear(0.33) transformation strain. Interfacial energy is 0.1 J/m²

ΔG_{chem}, J/m³	$r_{crit,}$ nm	$\alpha_{crit,}$ nm	ΔE_{ξ}, J	ΔE_{τ}, J	$\Delta E_{elastic}$, J	$\Delta E_{surface}$, J	ΔG_{crit}, J	$\Delta G_{crit}/k$T at 500K
-4. 10^{8}	0.63	0.78	3.99 10^{-20}	0	3.99 10^{-20}	4.24 10^{-19}	1.41 10^{-19}	20.5
-3. 10^{8}	0.89	0.72	9.98 10^{-20}	0	9.98 10^{-20}	8.25 10^{-19}	2.75 10^{-19}	39.84
-2. 10^{8}	1.51	0.64	3.77 10^{-19}	0	3.77 10^{-19}	2.22 10^{-18}	7.39 10^{-19}	107.1
-1. 10^{8}	4.09	0.47	4.06 10^{-18}	0	4.06 10^{-18}	1.42 10^{-17}	4.72 10^{-18}	683.8
-4. 10^{8}	7.33	0.07	4.83 10^{-19}	2.14 10^{-17}	2.19 10^{-17}	3.43 10^{-17}	1.14 10^{-17}	1657
-3. 10^{8}	12.94	0.05	1.52 10^{-18}	6.75 10^{-17}	6.90 10^{-17}	1.06 10^{-16}	3.55 10^{-17}	5138
-2. 10^{8}	29.01	0.03	7.72 10^{-18}	3.42 10^{-16}	3.50 10^{-16}	5.32 10^{-16}	1.77 10^{-16}	2.57 10^{4}
-1. 10^{8}	115.60	0.02	1.23 10^{-16}	5.46 10^{-15}	5.59 10^{-15}	8.40 10^{-15}	2.81 10^{-15}	4.07 10^{5}

- Elastic energy contribution to activation barrier due to the shear is of the same order of magnitude as an interfacial energy. Overall barrier is 2 orders higher if the shear is not accommodated at nucleation stage.
- Thus, direct nucleation of single-layered nucleus without accommodation of shear is **impossible**.

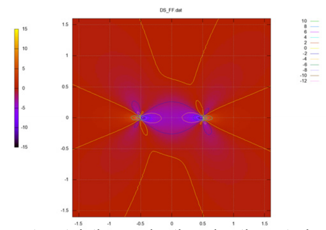


More detailed numerical estimates of the activation energy, using MD [5] data for interfacial energy and rigorous numerical solution for elastic energy shows that one-layer θ′ precipitates are energetically **favoured** without considering the shear, but never observed experimentally (only associated with a/2<100> dislocation loops), which supports the existence of shear component in transformation strain

5 Assisted nucleation

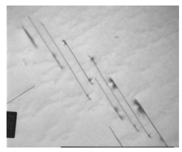
We here considered two cases of assisted nucleation:

- nucleation on a/2<100> dislocation loop, which helps to accommodate the shear component of the transformation. Below is an interaction energy map between the nucleus and the loop.

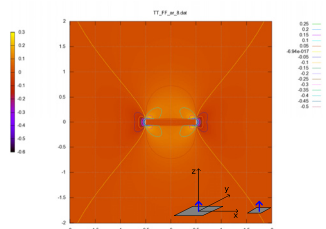


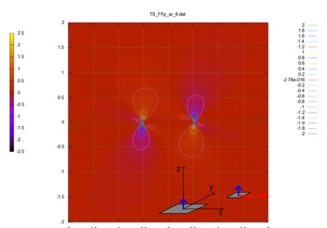
Map of the interaction energy density shows strong negative interaction of the loop with the nucleus, when the latter is placed close to the edge and inside the loop. So formation of a particle where shear is accommodated by the dislocation of appropriate Burgers vector is the easiest energetic path.

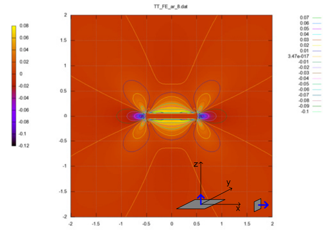
- autocatalytic nucleation in the strain field of the large, self-accommodated particle

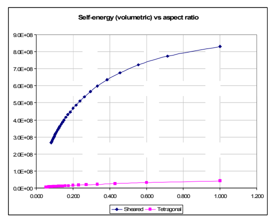


We ask is it possible to form a sheared nucleus in the field of existing particle, and if so, *where* should it happen? What is the role of shear in autocatalysis?









Results:

- self-accommodated variant (without shear) expected to form in-plane with existing particle (which differs from conclusion of Perovic et. al. [6])
- sheared nucleus, although has stronger interaction and spatially explains well formation of inclined parallel stacks of precipitates, is **unlikely** to form due to the significant self-energy barrier, which is not compensated by the interaction energy.

Conclusions

- Existing models of transformation mechanisms recognizing shear are in good qualitative and quantitative agreement with experimental data. Shear accommodation explains observed thickness of growing precipitates and their association with defects
- Autocatalytic nucleation requires further investigation, and apparently is not caused by the formation of the sheared nucleus in the field of the pre-existing particle. Phase-field modeling is expected to reveal the interplay between elastic interaction benefit for nucleation and reduced supersaturation of matrix due to solute depletion.

Acknowledgements

Yury Kryvasheyeu would like to acknowledge financial support provided by Monash University (Monash Graduate Scholarship) and Australian Government (International Postgraduate Research Scholarship)