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Reduction in the thermodynamic nucleation barrier via the heteroepitaxial recrystallization mechanism

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ABSTRACT

A new recrystallization mechanism characterized by the formation of a coherent γ shell around a primary γ' particle has been reported in superalloys [Charpagne et al. *J. Alloy Compd.* 688 (Part B) (2016) 685–694]. In the present work, the thermodynamics of nucleation by this mechanism are investigated, considering the stored deformation energy, interfacial energy, and elastic misfit. It is demonstrated that under realistic conditions, growth of any nucleus formed on a primary γ' particle is thermodynamically favorable regardless of size.

The control of grain size during thermomechanical processing of nickel-base superalloys is critical for obtaining the necessary mechanical properties, particularly the combination of creep and fatigue resistance required in the aerospace and power-generation industries [1]. As such, there has been substantial academic and practical interest in microstructural evolution during recrystallization and grain growth [2–6].

Recently, a new recrystallization mechanism has been described by Charpagne et al. in several polycrystalline nickel-base superalloys having low lattice misfit [7,8]. In their reported mechanism, coherent near-equiaxed γ shells form around pre-existing primary γ' particles during slow cooling after heat treatment via inverse precipitation prior to deformation. These shells are expected to be unstable at high temperature, dissolving during subsequent static heat treatment near the γ' solvus. However, during hot deformation, some of these γ shells grow driven by stored dislocation energy in what these authors term "heteroepitaxial recrystallization (HeRX)". A schematic representation of this mechanism is shown in Fig. 1. The authors report that this mechanism is active at low plastic strains. Above a threshold strain of approximately 0.6, the HeRX mechanism is gradually replaced by conventional discontinuous dynamic recrystallization (DDRX) with nucleation occurring primarily at pre-existing high angle grain boundaries.

The observation of this mechanism at small deformations—and consequently at low values of stored strain energy—is of particular interest, as it implies the nucleation barrier has been significantly reduced. In classical thermodynamic analyses of recrystallization (e.g. [9]), the volumetric driving force from stored energy of deformation is small in comparison to the surface energy penalty for the newly recrystallized grain. This results in large values of the critical nucleus size, on the order of 500 nm in diameter.

In contrast, during the HeRX mechanism the surface energy penalty may be mitigated by coherently templating γ recrystallization off incoherent γ' particles already present in the microstructure. In the present work, the various energetic contributions to HeRX nucleation are investigated under the assumption that a large primary γ' particle can be treated as a pre-existing nucleus for γ recrystallization. While Charpagne et al. describe inverse precipitation as a necessary component of the HeRX process [7,8], the present model considers nucleation in the absence of a pre-existing γ shell. The contribution and potential necessity of inverse precipitation to the HeRX phenomenon are discussed below.

An analytical model was developed to describe the thermodynamics of a spherical recrystallization nucleus formed via the HeRX

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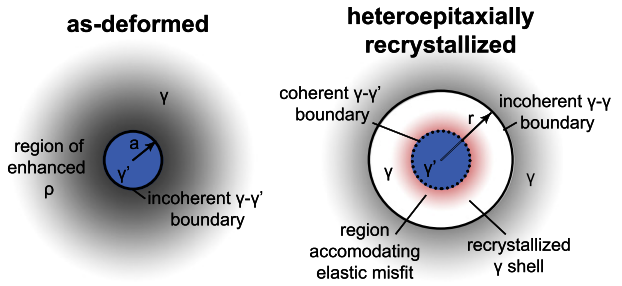

Fig. 1. Schematic representation of the HeRX nucleation mechanism.

mechanism, accounting for surface energy, stored energy of deformation, and elastic misfit strain energy. The total free energy of the nucleus is given by:

$$\Delta G^{total} = \Delta G^{surface} - \Delta G^{RX} + \Delta G^{elastic} \tag{1}$$

where $\Delta G^{surface}$ is the total surface energy penalty for the increase in surface area associated with the formation of the coherent γ shell, given by:

$$\Delta G^{surface} = 4\pi(r^2 - a^2)\gamma_b \tag{2}$$

In this equation, γ_b is the energy of a general high angle grain boundary between the γ phase grains, a is the radius of the γ' particle, and r is the total radius of the γ' particle and its coherent γ shell. It is assumed that the energy of an incoherent $\gamma-\gamma'$ interface is equal to that of a $\gamma-\gamma$ grain boundary.

The volumetric driving force for recrystallization can be approximated as the elastic energy of the dislocations stored during deformation which would be eliminated upon recrystallization. Therefore it can be calculated as the dislocation energy per unit volume multiplied by the volume of the coherent γ shell:

$$\Delta G^{RX} = \left(\frac{4}{3}\pi(r^3 - a^3)\right)\left(\frac{Gb^2}{2}\Delta\rho\right) = \frac{2}{3}\pi(r^3 - a^3)Gb^2\Delta\rho \tag{3}$$

In this expression, G is the shear modulus of the γ phase, b is the magnitude of the burgers vector in the γ phase, and $\Delta\rho$ is the difference in dislocation density between the deformed and recrystallized states.

The final term is the elastic energy due to the lattice mismatch between the primary γ' particle and the coherent γ shell. In this simple treatment, the particle is considered as a spherical Eshelby inclusion in an infinite isotropic medium [10,11]. While more sophisticated treatment is possible, it will be shown subsequently that the elastic contribution is quite small and the added complexity is largely unnecessary. The elastic strain energy in the volume V can be calculated as:

$$\Delta G^{elastic} = \frac{1}{2}\int_{V_{shell}} \sigma_{ij}\varepsilon_{ij}dV \tag{4}$$

The stress (σ_{ij}) and strain (ε_{ij}) fields under the assumptions outlined above are well-established and the derivation may be found elsewhere [12]. The resulting expression can be reduced to terms of the total radius of the HeRX grain:

$$\Delta G^{elastic} = \frac{2a^6E\left(\frac{1}{r^3} - \frac{1}{a^3}\right)(\delta - 2\delta\nu)}{27(\nu-1)^2(\nu+1)} \tag{5}$$

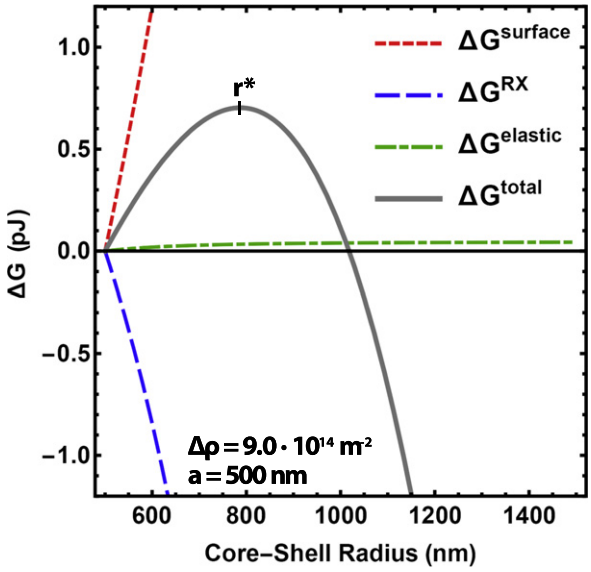

Fig. 2. Contributions to the free energy of a recrystallization nucleus, including contributions from stored deformation energy, elastic misfit energy, and surface energy penalty for a given set of parameters.

In this expression, E and ν are the Young's modulus and Poisson's ratio of the γ phase and δ is the $\gamma-\gamma'$ misfit. The elastic contribution to the free energy goes to zero when $r \to a$.

Substituting Eqs. (5), (3), and (2) into Eq. (1), the following expression for ΔG^{total} is obtained:

$$\Delta G^{total}(r) = 4\pi(r^2 - a^2)\gamma_b - \frac{2}{3}\pi(r^3 - a^3)Gb^2\Delta\rho + \frac{2a^6E\left(\frac{1}{r^3} - \frac{1}{a^3}\right)(\delta - 2\delta\nu)}{27(\nu-1)^2(\nu+1)} \tag{6}$$

The total change in free energy as a function of core-shell radius and the relative contribution of each term is shown in Fig. 2 for the material parameters given in Table 1. Under these conditions, the critical radius r^* is relatively large and successful nucleation is unlikely due to the high surface energy penalty and low volumetric driving force. However, for the assumed low misfit value, 1%, the relative contribution of elastic strain energy is much smaller than the magnitude of the interfacial energy or the volumetric driving force. This is true for all considered values of a and $\Delta\rho$. The alloys in which the HeRX mechanism has been reported all have misfit values well under the presently considered 1% and as low as 0.02% [7,8]. These misfits are also reported to decrease at elevated temperatures [13], making the contribution of elastic strain energy effectively negligible

Table 1
Parameters used for model of heteroepitaxial nucleation of recrystallization. The misfit is selected as an upper bound value, while the boundary energy, burgers vector, and elastic constant values are near those for pure Ni [14].

Parameter	Symbol	Value
Difference in dislocation density	$\Delta\rho$	*Varied*
γ' particle radius	a	*Varied*
Lattice misfit	δ	1%
Boundary energy	γ_b	866 mJ/m^2 [15]
Shear modulus	G	76 GPa
Burgers vector length	b	248.9 pm
Poisson's ratio	ν	0.31