



Modeling of the mutual effect of dynamic precipitation and dislocation density in age hardenable aluminum alloys



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ABSTRACT

A model has been proposed to capture the complex strain rate effect on dynamic precipitation of GP zones in an age-hardenable aluminum alloy. The contributions of vacancies and dislocations to dynamically formed GP zones have been specified in the model. It has been demonstrated that the proposed model is capable for predicting the contribution of each dynamic precipitation mechanisms, accurately, which are acting during deformation. Furthermore, the vacancy and dislocation evolutions during deformation have been considered in this modeling. The effect of strain rate by considering different mechanisms of dynamic precipitation of GP zones has been studied and confirmed by experimental data reported in the work of other researchers. Both experimental results and model outputs demonstrate that at high strain rate regime, strain rate dependency of dynamic precipitation is increased and in comparison with vacancy-assisted nucleation, dislocation-assisted nucleation of GP zones is encouraged. In this study, the mutual effects of dislocation density and dynamic precipitation have been considered. Outputs of model demonstrate that there is a weak negative strain rate sensitivity in the age-hardenable supersaturated aluminum alloy.

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1. Introduction

When a solution treated age-hardenable aluminum alloy system is subjected to a deformation process, it is well known that the solution treated structure is decomposed and dynamic precipitation can occur [1–8]. Due to profuse dynamic precipitation at room temperature, pronounced hardening is observed during deformation [4,6,9]. Deschamps et al. [9] depicted that dynamic precipitation in supersaturated Al-Zn-Mg results in very high levels of work hardening which is retained to large strains and increases the flow stress to very high levels (700 MPa) in modest strain increments (30%). The phenomenon of dynamic precipitation is closely related to dynamic strain ageing (DSA), because of solute clustering on dislocations and when the dislocations break free from the solute drag, the clusters left behind can nucleate precipitate [5,9]. The occurrence of precipitation through deformation is a very complicated situation. During plastic straining, there is a competition between different mechanisms. The accelerated nucleation may be owing to the presence of dislocations in the microstructure [4,10] or

may be owing to strain-induced non-equilibrium vacancies [6,11]. Thus, dynamic precipitation occurs due to either enhanced diffusion by vacancy, pipe diffusion or rearrangement at the dislocation cores [9].

There are few studies on the modeling of dynamic precipitation in age-hardenable aluminum alloys and no computation has been carried out [4,10]. Hutchinson et al. [4] observed pronounced cyclic hardening in under-aged Al-Zn-Mg-(Cu) due to room temperature dynamic precipitation of Guinier-Preston (GP) zones. They deduced that the accelerated formation of GP zones is due to the strain-induced excess vacancies that the concentration of these vacancies reaches a steady state very quickly [4]. By considering the effect of steady state excess vacancy content, they illustrated no effect of strain rate on the GP zones nucleation rate with respect to strain [4]. Deschamps et al. [10] estimated dynamic precipitation kinetics of GP zones in supersaturated Al-Zn-Mg-Cu alloy by a model which described DSA. In a specific range of strain rate at room temperature, dynamic precipitation of GP zones can lead to negative strain rate sensitivity (SRS) and Portevin-Le Châtelier (PLC) effect [10]. The aim of their model was only to represent the strain rate effect on the dynamic precipitation and no computation has been done [10]. Moreover, the mutual effect of dynamic precipitation and dislocation evolution has not yet been modeled. The

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second-phase particles and strain rate are also two important controlling parameters for PLC effect. For example, the coherent nanoscale $\text{Al}_3(\text{Sc,Zr})$ particles in Al-Mg alloy can change the flow stress curve behavior in this alloy [12,13]. Simar et al. [14,15] investigated the effect of dynamic precipitation on the work hardening of 6xxx aluminum alloys. The apparent effect of dynamic precipitation is an increase in dislocation storage and Simar et al. [14,15] considered this effect by adding a parameter which represents the effect of dynamic precipitation on the work hardening.

In this study, a comprehensive model for dynamic precipitation has been developed. Prior models only describe the effect of vacancy and dislocations on the dynamic precipitation, separately, but in the presented model the dislocation and vacancy evolutions during plastic deformation have been considered. In this model, to consider the effect of strain rate on the dynamic precipitation of GP zones both vacancy and dislocation-assisted nucleation have been attended and for condition with no strain rate effect on the dynamic precipitation just vacancy-assisted mechanism has been considered. Also, dislocation evolution during plastic deformation and the effect of dynamic precipitation on the dislocation density have been considered.

2. Model description

2.1. Dynamic precipitation model

In this part, dynamic precipitation of GP zones of supersaturated or under-aged aluminum alloys during deformation is modeled by classical nucleation theory. In this modeling, the size of dynamically formed GP zones is constant (4–5 Å) during different levels of strain because the GP zones are shearable particles and there is a competition between the diffusion control growth and precipitates fragmentation by shearing into many small pieces [4]. Based on classical nucleation theory, the nucleation rate during straining can be written as [4]:

$$\frac{dN}{d\varepsilon} = \frac{N_0 \beta^* Z}{\dot{\varepsilon}} \exp\left(-\frac{\Delta G^*}{kT}\right) \quad (1)$$

where N_0 , ε , $\dot{\varepsilon}$, k , T , β^* , Z and ΔG^* are the number of nucleation sites, strain, strain rate, Boltzmann's constant, temperature, kinetics attachment factor, Zeldovich factor and activation energy for nucleation, respectively.

Enhanced dynamic precipitation of GP zones can be assumed by dislocation-assisted process and excess vacancy-assisted process which promotes diffusion. Some authors [10] suggested dislocation-assisted process for dynamic precipitation; in fact they introduce dislocations as heterogeneous nucleation sites. In contrast to this claim, Hutchinson et al. [4] and Han et al. [6] believed that since there is no strong dependency of dynamic precipitation on strain rate and the distribution of dynamically formed GP zones is extremely homogenous, so the dynamic precipitation process is caused by excess vacancy-assisted process, although the excess vacancy content is in relation with dislocation density. Also, Militzer et al. [16] suggested that excess vacancies are responsible for strain-induced precipitation.

In the present study, at first, dynamic precipitation of GP zones is considered as excess vacancy-assisted process and the evolution of excess vacancies during plastic straining can be investigated by Militzer formulation [16]. The excess vacancies evolution during deformation is given by [16]:

$$\dot{C}_v^{ex} = \dot{C}_v^{ex+} - \dot{C}_v^{ex-} \quad (2)$$

where \dot{C}_v^{ex+} and \dot{C}_v^{ex-} are the production rate and annihilation rate of excess vacancies, respectively. The production rate of excess vacancies is obtained by [16]:

$$\dot{C}_v^{ex+} = \chi \frac{\sigma \Omega}{Q_{vf}} \dot{\varepsilon} + \zeta \frac{c_j \Omega}{4b^3} \dot{\varepsilon} \quad (3)$$

where χ is a constant and equal to 0.1, σ is the stress level, Ω is the atomic volume, Q_{vf} is the vacancy formation energy, c_j is the thermal jog concentration, b is the Burgers vector and ζ is the neutralization effect produced by the presence of vacancy absorbing jogs [16]. Since, $c_j < 1$ at room temperature and here dynamic precipitation is considered at low temperatures, the second term of above equation is small in comparison with the first term and can be neglected (i.e. $\dot{C}_v^{ex+} = \chi \frac{\sigma \Omega}{Q_{vf}} \dot{\varepsilon}$).

The annihilation of excess vacancy occurs at grain boundaries and dislocations, so the expression of annihilation rate is given by [16]:

$$\dot{C}_v^{ex-} = D_v \rho C_v^{ex} + \frac{D_v}{g^2} C_v^{ex} \quad (4)$$

where D_v is the vacancy diffusivity, ρ is the dislocation density and g is the grain size. To sake of simplicity, the second term of Eq. (4) is small in comparison with the first term, so this term can be neglected (i.e. $\dot{C}_v^{ex-} = D_v \rho C_v^{ex}$). The evolution rate of excess vacancies can be expressed by the following equation [16]:

$$\dot{C}_v^{ex} = \chi \frac{\sigma \Omega}{Q_{vf}} \dot{\varepsilon} - D_v \rho C_v^{ex} \quad (5)$$

If vacancy annihilation distance is considered as $\lambda = \rho^{-1/2}$ and constant, the vacancy super saturation content (i.e. $\dot{C}_v^{ex} = 0$) can be obtained by [4]:

$$C_v^{ss} = \frac{\chi \sigma \Omega \lambda^2 \dot{\varepsilon}}{D_v Q_{vf}} \quad (6)$$

The kinetic attachment factor β^* is proportional to diffusivity of rate controlling solute atom (D_s) and can be written as $\beta^* = \Phi \frac{D_s C_v^{ex}}{C_v^{eq}} X_b$, where Φ , C_v^{eq} and X_b are the geometrical factor, equilibrium vacancy content and the mole fraction of solute in the matrix [4]. Here, the upper extreme of excess vacancy content is considered (i.e. $C_v^{ex} = C_v^{ss}$) and by substituting β^* in Eq. (1) the following equation can be derived:

$$\left. \frac{dN}{d\varepsilon} \right|_{vac.} = N_0 Z \Phi X_b \frac{D_s}{D_v C_v^{eq}} \frac{\chi \sigma \Omega \lambda^2}{Q_{vf}} \exp\left(-\frac{\Delta G^*}{kT}\right) \quad (7)$$

We know that dynamic precipitation can lead to negative strain rate sensitivity and this phenomenon is related to dislocations [10]. Thus, it is necessary to consider the effect of dislocations on the dynamic precipitation of GP zones. Deschamps et al. [10] considered waiting time of dislocations (t_w) at obstacles and during this time solutes concentrations build up on the dislocation. Based on Cottrell-Bilby law, at short waiting time, solute concentration on the dislocation (C_d) is proportional to $t_w^{2/3}$, but for simplicity, we can assume that nucleation rate during the waiting time t_w is proportional to solute concentration on the dislocation, thus:

$$\left. \frac{dN}{d\varepsilon} \right|_{disln.} = \frac{3}{4\pi} \frac{1}{r^3} \frac{k' \rho_m}{t_w^{1/3} \dot{\varepsilon}} \quad (8)$$

where k' and r are a proportionality constant and radius of GP zones, respectively, and ρ_m is the mobile dislocation density and it generally reaches a saturation value at low level of strain. By

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