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Grain growth jointly affected by immobile and mobile particles

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ABSTRACT

Grain growth under the influence of randomly distributed particles is studied by numerical simulation using Onsager's principle. It was found that at small initial volume fraction of particles, normal grain growth evolves, with its kinetic law depending on the particle dissolution rate and its rate affected by particle mobility. At large initial volume fraction of particles, abnormal grain growth develops whereas an increase in particle mobility can lead to evolution of normal grain growth instead. Results of the simulations describe the effects behind some experimental data, lacking an explanation so far. They also allow improving existing and develop new technological solutions in the field of grain structure control and design.

1. Introduction

In the course of normal grain growth, microstructure remains homogeneous while the mean grain size increases continually. In abnormal grain growth (AG), several large grains grow rapidly whereas the remainder of microstructure hardly changes, which results in the formation of non-homogeneous microstructure and in discontinuous increase in the mean grain size.

The presence of particles is often responsible for AG evolution. They also affect kinetics of both normal and abnormal grain growth. There are two alternatives of grain boundary (GB) interaction with particles. The first one is appearance of some drag force owing to GB's release from particles [1]. The second one is slowing down GBs motion owing to necessity to move together with particles [2]. To the best of our knowledge, there are no studies of grain growth under the combined effect of different versions of GB's retardation. Since grain growth, especially AG, readily develops under thermal instability of second phase (see, e.g. [3,4]), this work is aimed at the study of grain growth in the course of particle dissolution. The reasons for such a choice were the following. First, the drag force exerted by particles decreases because of their dissolution, which promotes grain growth. Second, in the course of dissolution, the particle radius decreases, which raises the fraction of particles able to migrate together with GBs. This study was performed by numerical simulation.

2. Model description

A statistical model [5] tracking changes in grain size distribution in the course of grain growth is applied. Grain growth is described by taking into consideration the displacements of boundaries between grains of various sizes, probabilities of the grain contact, and magnitudes of grain contact surface. The model allows describing the influence of drag forces from immobile particles as well as impacts of mobile particles and GB's junctions [6–8].

In the course of particle dissolution, their volume fraction f decreases with time t [9]:

$$f = f_0 \exp(-c_f t^{3/2}) \tag{1}$$

Since the number of mono-size particles per unit volume n_v remains constant, the particle radius is:

$$R = (3f/4\pi n_v)^{1/3} \tag{2}$$

It is assumed that the spatial distribution of particles is random and does not change with time.

Grain growth kinetics is affected by particles lying on GBs. Particles can be able to migrate together with GBs (further they are termed 'mobile') or detach from GBs ('immobile' particles). According to [10], a particle of radius R is able to move along with GB if the migration rate of the latter does not exceed

$$v^* = \pi R \gamma M_p \tag{3}$$

where γ is the GB energy and M_p is the particle mobility:

$$M_p = \delta D_s \Omega/(kT\pi R^4) = c_m/R^4 \tag{4}$$

δ being the 'diffusion thickness' of the particle/matrix interface, D_s

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– coefficient of interfacial diffusion, Ω – atomic volume [11]. If GB's migration rate is $\geq v^*$, particle behaves as immobile, in the opposite case – as mobile. The rate of GB's migration affected by immobile particles is [5]:

$$v_z = \gamma M_{gb}(1/D_j - 1/D_i - Z) \quad (5)$$

where M_{gb} is GB's mobility, D_j and D_i – diameters of the consumed and the growing grain, respectively ($D_j < D_i$), $Z = 1.5f/R$ – the multiplier in the expression for Zener's drag force [1]. Since v_z obeys the condition $v_z \geq 0$, it follows from Eq. (5) that immobile particles prevent a part of grains from growing. Mobile particles, in contrast, retard the growth of all grains through decreasing GB's effective mobility [12]:

$$v_m = \gamma M_{gb}(1/D_j - 1/D_i)/(1 + n_a M_{gb}/M_p) \quad (6)$$

where $n_a = 1.5f/\pi R^2$ is the number of particles per unit GB area. It is self-evident that GB's migration rate affected by particles can be either v_z or v_m. To decide between these options, the following condition is used in the model: particles behave as mobile if simultaneously $v_m < v^*$ and $v_m > v_z$. The former follows from Ref. [10], the latter–from Ref. [13], according to which only the processes in a system take place that lead to the maximum rate of the free energy dissipation. In all other cases, particles behave as immobile.

In the simulations, γ, M_{gb} and M_p were supposed to be identical for all GBs/particles and independent of time. Microstructure was described by the number-averaged grain diameter D and by the D_{max}/D ratio characterizing the inhomogeneity of grain sizes. AG was assumed to develop at $D_{max}/D > 5.0$. It starts at the point in time where the ratio, after reaching 5.0, continuously increases further. This made it possible to find the volume fraction V_A of abnormal grains and its time dependence. Since in the course of AG the magnitude of D_{max}/D first increases and then decreases, it was assumed that AG terminates at the instant when D_{max}/D becomes ≤ 5.0. If at this instant $V_A \approx 100\%$, we deal with a 'completed' AG when the parent fine-grained matrix is fully consumed by abnormal grains. At $V_A < 100\%$, the matrix is not entirely consumed; AG in this case is termed 'interrupted'. In both cases, normal grain growth takes place after AG termination.

3. Results and discussion

The impact of c_f upon R and Z is shown in Fig. 1. Over a period of 300 min, R decreases by ~10% at $c_f = 10^{-5}$ and by ~60% at $c_f = 10^{-4}$ whereas the corresponding Z reduces by ~15% and ~80%, respectively.

The influence of particle dissolution and mobility on normal grain growth was studied at small drag force. Fig. 2a demonstrates simulation results for $c_f = 10^{-5}$ while Fig. 2b – those for $c_f = 10^{-4}$. In each of them, kinetic curves appear to be similar whereas their shapes are different. Obviously, the latter is connected with different time dependences of the drag term Z (cf. Fig. 1). It was also found that, in both cases, kinetic curves practically coincide at $c_m = 10^{-5}$ and 10^{-4}. As to the other c_m magnitudes, it is seen that an increase in c_m increases the rate of the growth process. Fig. 2c additionally presents the growth kinetics at an increased R_0. Comparison with Fig. 2b shows that, as could be expected (see Eq. (4)), this decreases the rate of grain growth. At the same time, the shapes of kinetic curves in Figs. 2b and c are identical, which supports the above conclusion about the role of the time dependence of Z.

It is common practice to compare results on growth kinetics with the dependence

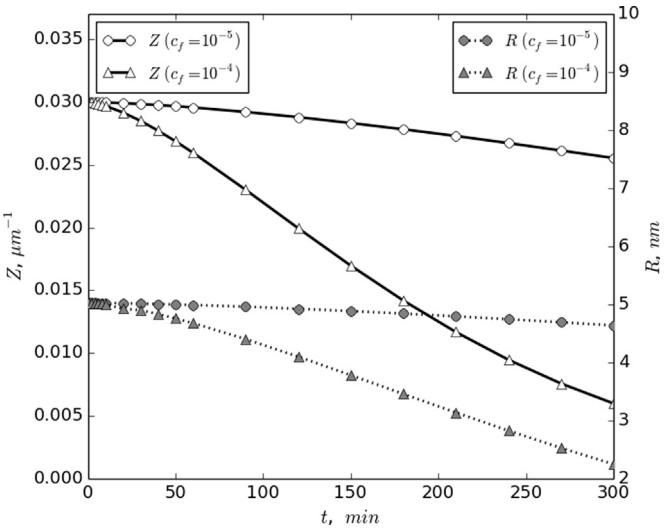

Fig. 1. Time dependences of R and $Z = 1.5f/R$ in the course of particle dissolution. $R_0 = 5$ nm, $f_0 = 0.01\%$, $Z_0 = 0.03$ μm^{-1}.

$$D = kt^{0.5} \quad (7)$$

derived for an ideally pure polycrystal with identical GB's properties and an identical growth law for all grains. Usually, the grain growth exponent n is < 0.5, which has been explained by the effect of GB's solute segregation. Kinetic curves in Fig. 2a approximately correspond to the parabolic dependence (7) with $n = 0.2$ at $c_m = 10^{-5}$ and 10^{-4}; an increase in c_m to 10^{-3} raises the time exponent to ~0.4 while at $c_m = 10^{-2}$ its magnitude reaches ~0.6. These results permit us to interpret an unexplained increase in the time exponent from 0.35 at 500 °C to 0.6 at 850 °C in a pure α-brass [14]. Following the common trend, an increase in n with temperature could be explained by decay of the solute segregation effect, but this cannot be applied to the data [14] because, according to the theory, n cannot exceed 0.5. As to our results, they perfectly explain the experimental data [14] as a whole if we take into account that GBs can be retarded by disperse particles always present in technical alloys and that both c_f and c_m are temperature dependent.

AG evolution was observed at f_0 magnitudes exceeding that leading to normal grain growth. The impact of particle dissolution alone on AG was studied at $c_m = 10^{-8}$, i.e. in the presence of practically immobile particles, and $c_f = 10^{-5}$. (The c_f magnitude was chosen with the intent to guaranty distinct particle dissolution (cf. Fig. 1).) A characteristic AG kinetics at $f_0 = 0.15\%$ shown in Fig. 3 was observed in a wide f_0 range. Large f_0 magnitudes lead to AG development at f_0 up to 0.25% and AG evolves completely. An increase in c_m reduces the tendency to AG and leads to its interruption, as shown by dotted line in Fig. 3, and even suppression. Fig. 4 shows that at $c_m = 10^{-4}$, AG gives way to normal grain growth at $f_0 > 0.18\%$ and at $c_m = 3 \cdot 10^{-4}$ even at ~0.10%. These data for the first time offer the opportunity to understand the AG interruption in zone-annealed ODS superalloys at high temperatures. AG in those alloys takes place at temperatures below certain limit, whereas at higher temperatures it ceases and normal grain growth evolves instead (see e.g. [15]). These results suggest that an increase in the annealing temperature and, consequently, an increase in particle mobility could prevent the AG evolution.

Before discussing the simulation results let us consider an important aspect of our model, namely, deciding between v_m and v_z. It is assumed in the model that grain growth evolves through the processes leading to the maximum rate of the free energy dissipation. (This principle was for the first time applied to GB motion in Ref. [16].) Situations with different possible paths of