Mechanism of grain growth in aluminium, cadmium, lead and silicon

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Abstract : A simple model has been developed to evaluate the mechanism of grain growth in Al, Cd, Pb and Si for various annealing times and annealing temperatures based on the diffusion of atoms from one grain to another. Our numerical values of grain size have been compared with the available experimental results. There exists a fairly satisfactory agreement between them The above model has been extended to calculate the grain size distribution as a function of annealing time and annealing temperature. The results are discussed in detail.

1. Introduction

Polycrystalline metals have been used in all engineering application. Recently the study of mechanical properties has moved away from the processes which occur inside the individual grain to those which are governed by the boundaries between the grains. Most of the properties such as high temperature creep, superplasticity, recrystallisation, yielding and embattlement all depend strongly on effects at grain boundaries. There are numerous variables which can affect the structure and properties of a grain boundary. These include the crystallographic parameters which describe the orientation of the adjoining crystals and the interface between them. The grain boundary is an internal surface, in a single phase material, across which there is a discontinuity of crystal orientation. It shares in common with interphase surfaces, the property of a free energy per unit area [1]. At elevated temperatures, it is able to move under driving forces by invading one grain and enlarging the other in its wake. Recently, powerful theoretical

and experimental techniques have been developed to investigate the grain boundary migration.

The phenomenon of grain boundary migration occurs when a grain boundary is subjected to a driving force sufficient to cause motion of the boundary. The resultant boundary migration will be such as to cause a reduction in the free energy of the system. Boundary migration is a thermally activated process and hence the rate at which a boundary migrates under the influence of a given driving force is strongly temperature dependent [2–5]. In this paper, a kinetic model was proposed to understand the grain growth mechanism in Al, Cd, Pb and Si for various annealing time and temperature.

2. Theory

Our kinetic model is based on the diffusion of atoms from one grain to another. Using this, we have determined the grain size distribution in Al, Cd, Pb and Si. The driving force for the movement of atoms from one grain to another is related to the grain boundary energy and radius of the grain. The difference of chemical potential between the two adjustant grains, which is the driving force for the grain growth is given by [6]

$$D = \frac{Fa^3E}{r},$$ (1)

where F is a constant related to the geometric shape of the grains (for spherical grains $F = 2$), E is the grain boundary energy, a is the lattice constant and r is the grain size.

From basic rate theory, the net rate of atomic transfer across the boundary (from lattice sites of one grain to those of a neighbour) is given by [7]

$$A = \frac{D_g}{W^2}\left[1 - \exp\left(\frac{-D}{kT}\right)\right],$$ (2)

where D_g is the self diffusion constant of the atoms across the grain boundary, k is the Boltzmann's constant, T is the annealing temperature and W is the thickness of the grain boundary. The rate of boundary motion is given by the product of the net rate of atomic transfer across the boundary and the thickness. Therefore, the grain growth rate becomes

$$\frac{dr}{dt} = AW = \frac{D_g}{W}\left[1 - \exp\left(\frac{-D}{kT}\right)\right].$$ (3)

Expanding the exponential, neglecting the cube and higher powers of D/kT and using eq. (1)

$$\frac{dr}{dt} = \frac{2D_g}{W}\left(\frac{L}{r}\right)\left[1 - \left(\frac{L}{r}\right)\right],$$ (4)

where $L = \frac{Fa^3E}{2kT},$

Integrating eq. (4)

$$2D_g \, Lt/W \; = \; \left[(r-L)^2/2 \, + \, 2L(r-L) \, + \, L^2 \, \log(r-L)\right]_{r_0}^{r}, \tag{5}$$

where t is the time of annealing and r_0 is the initial grain size. Expanding the right hand side of eq. (5), applying the limits and neglecting the cube and higher power of L, since L is very small compared to the value of r_0, we get

$$r \; = \; \left(L^2 \, + \, 4D_g \, Lt/W \, + \, r_0^2 \, + \, 2Lr_0\right)^{1/2} \, - \, L. \tag{6}$$

It is noted that the grain size is directly proportional to the square root of annealing time as reported earlier [6–12]. This model has been extended to evaluate the grain size distribution for different annealing time and annealing temperatures. By introducing a dimensionless variable known as relative grain size, $V = r/r_{cr}$ in eq. (4), and simplifying

$$\frac{dV^2}{d\tau} \; = \; \left[(4D_g \, L/W)\left(1 - \frac{L}{Vr_{cr}}\right)\frac{dt}{dr_{cr}^2} \, - \, V^2\right], \tag{7}$$

where $1/d\tau = r^2/dr_{cr}^2$, r_{cr} is the average grain size and $d\tau$ represents the time.

$$\frac{dV^2}{d\tau} \; = \; \left[G\left(1 - \frac{H}{V}\right) - V^2\right], \tag{8}$$

where $G = (4D_g \, L/W) \, dt/dr_{cr}^2$ and $H = L/r_{cr}$.

$$\frac{dV}{d\tau} \; = \; \frac{1}{2V} \left[G\left(1 - \frac{H}{V}\right) - V^2\right]. \tag{9}$$

The eq. (9) has been solved to determine the steady state grain size distribution during normal grain growth mechanism, using the Hillert's [9] approach. The whole distribution of the individual grain size during the steady state is given by

$$P(V) \; = \; \frac{1}{2}\exp(-\beta\psi/2)/[dV/d\tau], \tag{10}$$

where β is a constant ($\beta = 2$ for two dimensional system, $\beta = 3$ for three dimensional system) and

$$\psi \; = \; \int_0^V dV/(-dV/d\tau). \tag{11}$$

From eqs. (9) and (11)

$$\psi \; = \; \left[\frac{2}{3}\log(V^3 - GV + GH)\right]_0^V \, + \, Y. \tag{12}$$

where

$$Y \; = \; \frac{2G}{3} \int_0^V \frac{dV}{(V^3 - GV + GH)}.$$

Numerical integration method has been followed to determine the value of Y. Substituting the values of $dV/d\tau$ and ψ from eqs. (9) and (12) respectively in eq. (10), we get

$$P(V) = \frac{\beta V^2}{(V^3 - GV + GH)[(V^3 - GV + GH)/GH]^{\beta/3} \exp(\beta Y/2)}. \qquad (13)$$

Eq. (13) gives the grain size distribution.

3. Results and discussion

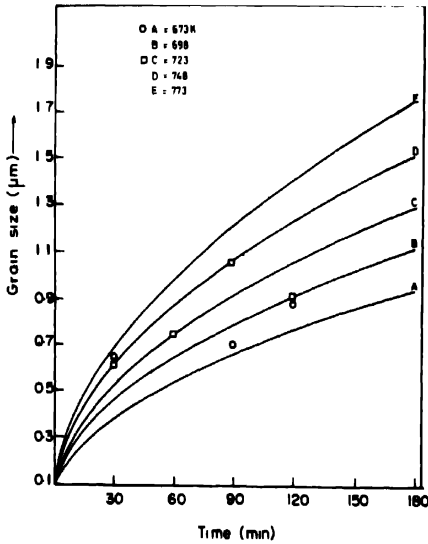Eqs. (6) and (9) have been used to evaluate the numerical values of grain size distribution for different time of annealing and annealing temperature.

Figure 1. Variation of grain size *vs* annealing time in Al for different annealing temperatures.
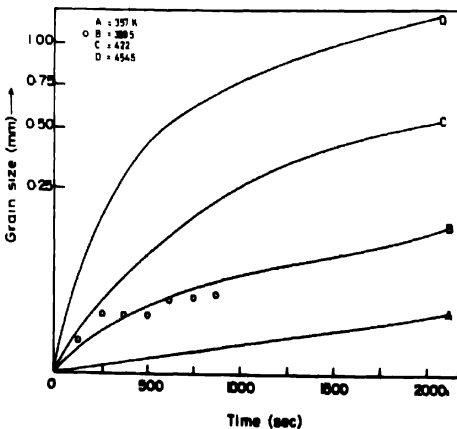
Figure 2. Variation of grain size *vs* annealing time in Cd for different annealing temperatures.

Figure 1 shows grain size *vs* annealing time in Al for different annealing temperatures. Experimentally reported results [13] are also plotted in the Figure. Figure 2 is
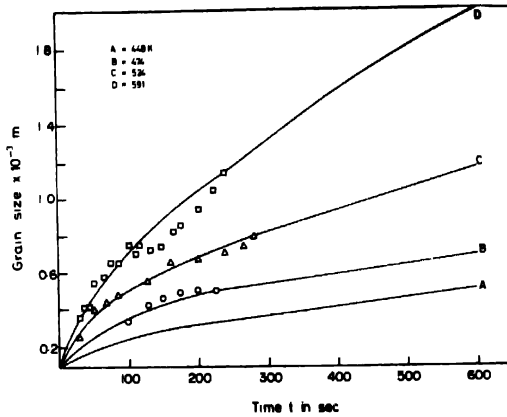

Figure 3. Variation of grain size *vs* annealing time in Pb for different annealing temperatures.
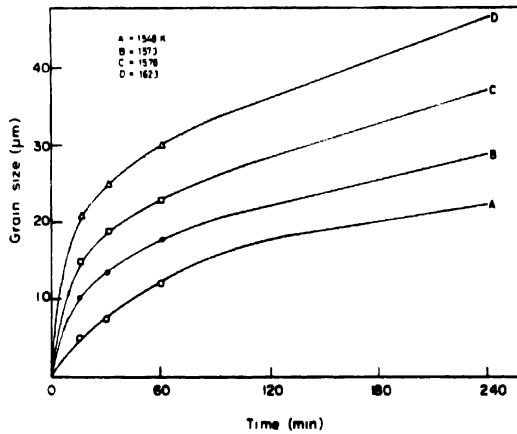

Figure 4. Variation of grain size *vs* annealing time in Si for different annealing temperatures.

plotted between grain size and annealing time in Cd for different annealing temperature with the experimental values [14]. Figure 3 is drawn for grain size and annealing time in Pb for different annealing temperatures. Experimental points [15] are also shown in the Figure. Figure 4 is plotted between grain size and annealing time in Si for various annealing temperatures and experimental results [16]. From the numerical results it can be concluded

that grain size increases with annealing time and annealing temperature and there is a fairly satisfactory agreement between the experimental and our theoretical results.
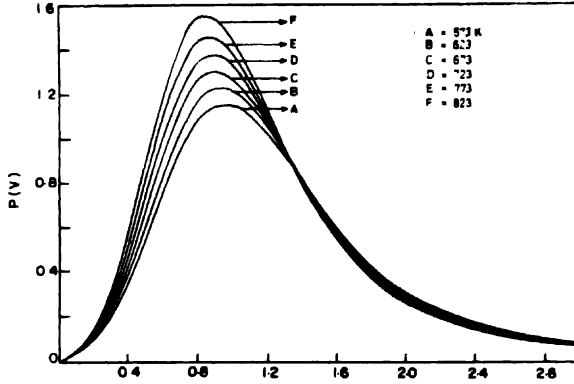

Figure 5. Variation of grain size distribution *vs* relative grain size in Al for different annealing temperatures for three hours of annealing time.
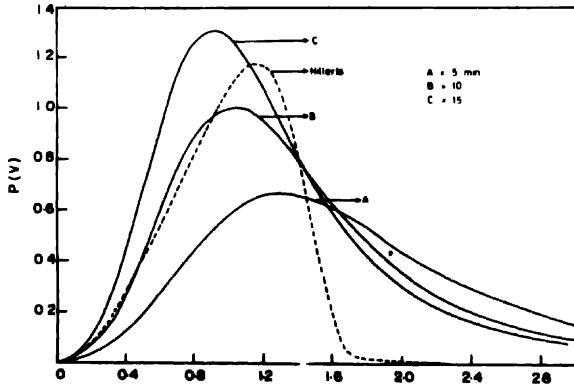

Figure 6. Variation of grain size distribution *vs* relative grain size in Cd for different annealing times for the annealing temperature of 389.5 K.

Figure 5 shows grain size distribution *vs* relative grain size in Al for different annealing temperatures and for three hours of annealing. Figure 6 is drawn grain size distribution *vs* relative grain size in Cd for different annealing times and for the annealing temperature of 389.5 K. The dotted line shows the Hillert's result. Figure 7 is drawn for grain size distribution and relative grain size in Pb for five different annealing temperatures and three minutes of annealing time. Figure 8 is plotted between grain size distribution and relative grain size in Si for different annealing times and annealing temperature of 1548 K. From the results, we observe that the grain size distribution gradually increases with increases of relative grain size, attains a maximum and with further increase of relative

grain size, the grain size distribution decreases. The maximum point also increases with annealing time and annealing temperature. There are no experimental reports in the literature for the grain size distribution.
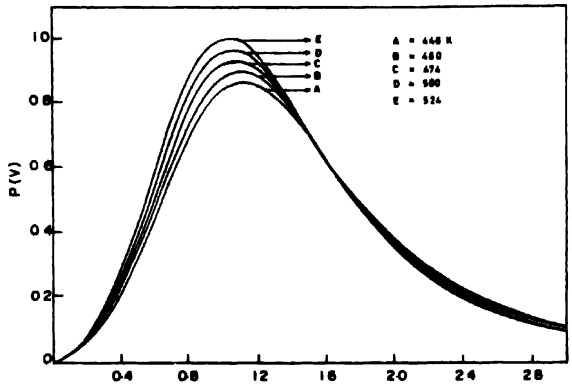

Figure 7. Variation of grain size distribution *vs* relative grain size in Pb for different annealing temperatures and three minutes of annealing time.
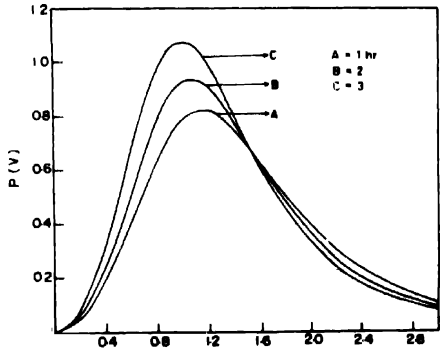

Figure 8. Variation of grain size distribution *vs* relative grain size in Si for different annealing times and annealing temperature of 1548 K.

4. Conclusion

From the numerical results, we conclude that the grain size and their distributions in materials like Al, Cd, Pb and Si, increases with the increase of annealing times and annealing temperatures. It is due to the large number of atoms segregated at the grain boundaries.

Acknowledgment

References

[1]   W W Mullins *Acta. Metal.* **4** 421 (1956)

[2]   C J Simpson, W C Winegasrd and K T Aust *Grain Boundary Structure and Properties* eds G A Chadwick and D A Smith (London : Academic) p 201 (1976)

[3]   D J Jensen *Acta. Metallurg. Mater.* **43** 4117 (1995)

[4]   D C Vanaken, P E Krajewski, G M Vyletel, J E Allison and J W Jones *Metallurg. Mater. Trans.* **26A** 1395 (1995)

[5]   V Y Gortsman and Q R Birringer *Scr. Metallurg. Mater.* **30** 577 (1994)

[6]   S Kalainathan, R Dhanasekaran and P Ramasamy *Thin Solid Films* **163** 383 (1988)

[7]   C V Thomson *J. Appl. Phys.* **58** 763 (1985)

[8]   L Mei, R River, Y Kwart and R W Dutton *J Electrochem. Soc.* **129** 1791 (1982)

[9]   M Hillert *Acta. Metal.* **13** 763 (1965)

[10] S Kalainathan, R Dhanasekaran and P Ramasamy *J. Crystal Growth* **104** 250 (1990)

[11] S Kalainathan, R Dhanasekaran and P Ramasamy *J. Electron. Mater.* **19** 1135 (1990)

[12] S Kalainathan, R Dhanasekaran and P Ramasamy *J. Mater. Sci. : Materials in Electron.* **2** 98 (1991)

[13] S S Iyer and C Y Wong *J. Appl. Phys.* **15** 4594 (1985)

[14] E A Grey and G T Higgins *Scr. Metal.* **6** 253 (1972)

[15] C F Bolling and W C Winegard *Acta. Metal.* **6** 283 (1958)

[16] G C Jain, B K Das and S P Bhattacherjee *Appl. Phys. Lett.* **33** 445 (1978)