

## The Mechanism of Grain Boundary Migration in Aluminum Bicrystals

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### ABSTRACT

The effect of high pressure on the migration rate of grain boundaries (GBs) was studied in aluminum bicrystals. The boundaries were of the tilt type, with  $\langle 111 \rangle$ ,  $\langle 100 \rangle$  and  $\langle 110 \rangle$  tilt axes. For each tilt axis at least two boundaries were studied, one with a periodic and another one with a non-periodic structure. It was found that for the  $\langle 111 \rangle$  and  $\langle 100 \rangle$  boundaries the activation volume  $V^*$  for migration was independent of both the activation energy and the misorientation and was close to the atomic volume ( $\Omega$ ). For the four  $\langle 110 \rangle$  boundaries investigated  $V^*$  was proportional to the activation energy and was in the range 1.2-3.1 $\Omega$ . We conclude that in analogy to the concept of compensation temperature, the above results speak for the idea of compensation pressure, a characteristic property of the activated cluster formed during atomic jumps. The value of this pressure permits to assess the pressure level inside the activated cluster formed during the transfer of atoms across the boundary and to get new insight in the mechanisms of grain boundary migration.

### 1. INTRODUCTION.

It is known since more than 50 years that there is a correlation between the pre-exponential factor of the diffusion coefficient  $D$  and the activation enthalpy [1]:

$$\ln(D_0) = \frac{H^*}{T} \quad (1)$$

Here  $D_0$  is the pre-exponential factor and  $H^*$  is the activation enthalpy. The correlation holds for instance when different impurities diffuse in a constant matrix [cf.1]. Eq.(1) will be hereafter called *compensation relationship*. Zener explained the above relationship as follows: since  $\ln(D_0) = S^*/R$ , eq.(1) reflects the fact that the entropy of the activated cluster formed at the

saddle point configuration of the system is proportional to the enthalpy:  $\Delta S^* = \Delta H^*/T$ . Zener assumed the jump to be slow comparing to the time for equilibration of the activated cluster with the matrix. The activation entropy is the derivative of the free energy of activation:  $\Delta S^* = -dG/dT$ .  $G^*$  was assumed to change with temperature as the shear modulus. Therefore:

$$\Delta S \cong \beta \left( \frac{H}{T_m} \right) \quad (2)$$

$$\beta = -d \left( \frac{\mu(T)}{\mu} \right) / d \left( \frac{T}{T_M} \right) \quad (3)$$

Here  $\beta$  is the effect of temperature on the normalized shear modulus. However, it is known now that the compensation rule holds also for grain boundary diffusion and migration when the grain boundary misorientation is varied [3-7]. In that case the elasticity arguments of Zener do not apply and we believe that the compensation rule reflects deeper thermodynamic relationships. In particular, it was proposed that formation of the activated cluster is equivalent to a local phase transformation (cf.ref. 3-7). The term "compensation temperature"  $T_c$  was introduced [3-7]:

$$S^* = \frac{H^*}{T_c} \quad (4)$$

As can be seen, eq.(2) is a special case of eq.(4) with  $T_c = \beta T_m$ . For  $T = T_c$  all boundaries have the same diffusion coefficient or migration rate. Recent investigations of the pressure effect on grain boundary diffusion [3] have led to the concept of compensation pressure. We will illustrate this point based on recent results of investigations of the effect of pressure on GB migration [6].

## 2. CORRELATION BETWEEN PRE-EXPONENTIAL FACTOR, ACTIVATION ENERGY AND ACTIVATION VOLUME FOR GRAIN BOUNDARY MIGRATION IN ALUMINUM BICRYSTALS.

In a recent paper [6] the pressure effect on the rate of migration of grain boundaries in aluminum bicrystals with well defined crystallographic orientation relationships was investigated. Fig.1 and 2 show the correlation we observed between pre-exponential factor and activation volume (fig.1) as well as between the activation volume and activation energy (fig.2). Inspection of the figures shows two kinds of linear relationships. For  $\langle 110 \rangle$  boundaries the activation volume and energy are proportional to each other. Also, the pre-factor is proportional to the activation volume. For the  $\langle 100 \rangle$  and  $\langle 111 \rangle$  tilt axes the pre-factor does not depend on  $V^*$  but depends on the activation energy [6]. Let us concentrate on the  $\langle 110 \rangle$  boundaries. Fig.1 provides another example of the "compensation relationship", where there is a linear relation between the pre-exponential factor and activation energy. However, in that case we have to do with compensation pressure  $P_c$  instead of temperature.  $P_c$  is defined as follows: expanding eq.4 and taking into account the term  $pV$ , eq.(5) yields.

$$S^* = \frac{H^*}{T_c} = \frac{Q^*}{T_c} + \frac{P_c V^*}{T_c} \quad (5)$$

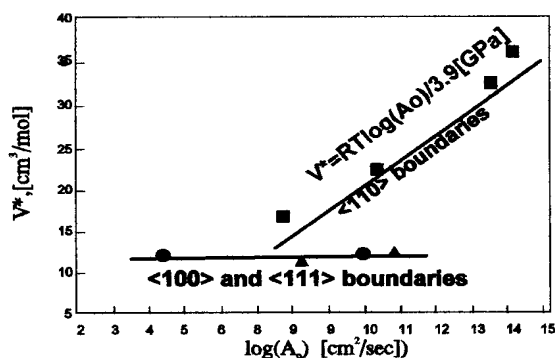


Fig.1. Correlation between pre-exponential factor and activation volume for grain boundary migration in Al bicrystals.

correspond therefore to the local temperature and pressure in the cluster (fig.3). The assumption of a phase transformation is crucial, because it permits to understand why all clusters have the same temperature and pressure, which in turn ensures the observed linear correlations. If this assumption is true, an increase of the volume of the cluster must be connected with an increase of its energy. In fact, from fig.2 it can be deduced that for  $\langle 110 \rangle$  boundaries  $E^* = PV^*$ , where  $P = 5.0(\pm 1.0)$  GPa. This value is close to  $P_c = 3.9(\pm 0.8)$  GPa. The close value of the two pressures speaks in favor of the idea that  $P_c$  is actually the pressure within the activated cluster. For the  $\langle 100 \rangle$  and  $\langle 111 \rangle$  boundaries  $V^*$  is constant and it is impossible to determine  $P_c$ .

#### 4. CONCLUSIONS FOR THE GRAIN BOUNDARY MIGRATION MECHANISM.

The  $E^*(V^*)$  relationship displays two branches, one corresponding to the  $\langle 110 \rangle$  tilt axis and one to the  $\langle 100 \rangle$  and  $\langle 111 \rangle$  tilt axes. Since the relation between activation volume and activation energy is different for these two branches, the migration mechanism must differ between  $\langle 110 \rangle$  and  $\langle 100 \rangle$  or  $\langle 111 \rangle$  tilt boundaries. In fact, migration of  $\langle 110 \rangle$  boundaries is characterized by large activation volumes, reaching  $3\Omega$ . At the same time the

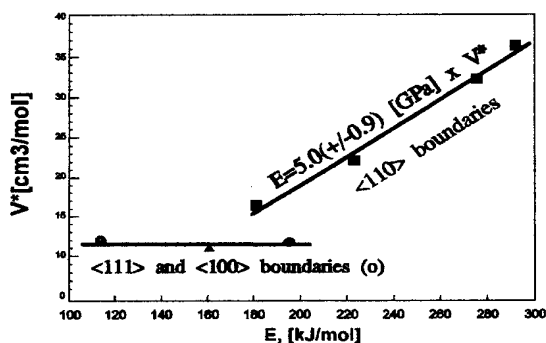


Fig.2. Correlation between activation energy and activation volume for grain boundary migration in Al bicrystals.

Therefore, there is a linear relationship between  $S^*$  and  $Q^*$ , where the proportionality constant is  $T_c^{-1}$  as well as between  $S^*$  and  $V^*$ , where the proportionality constant is  $P_c/T_c$ . For  $\langle 110 \rangle$  boundaries  $P_c = 3.9(\pm 0.7)$  GPa.

#### 3. INTERPRETATION IN TERMS OF THE HETEROPHASE FLUCTUATION THEORY.

According to the heterophase fluctuation theory [3,5], the activated cluster formed in the saddle point configuration is equivalent to a small nuclei of another phase corresponding to the locally disordered structure.  $T_c$  and  $P_c$

correspond therefore to the local temperature and pressure in the cluster (fig.3). The assumption of a phase transformation is crucial, because it permits to understand why all clusters have the same temperature and pressure, which in turn ensures the observed linear correlations. If this assumption is true, an increase of the volume of the cluster must be connected with an increase of its energy. In fact, from fig.2 it can be deduced that for  $\langle 110 \rangle$  boundaries  $E^* = PV^*$ , where  $P = 5.0(\pm 1.0)$  GPa. This value is close to  $P_c = 3.9(\pm 0.8)$  GPa. The close value of the two pressures speaks in favor of the idea that  $P_c$  is actually the pressure within the activated cluster. For the  $\langle 100 \rangle$  and  $\langle 111 \rangle$  boundaries  $V^*$  is constant and it is impossible to determine  $P_c$ .

pressure inside the activated cluster is of the order of 4-5 GPa. This is the order of magnitude of the pressure close to a dislocation core. At the same time, the  $\langle 110 \rangle$  direction is a close-packed direction in the fcc lattice. The high pressure inside the activated cluster could be understood in terms of whole segments of close packed rows of atoms in one grain jumping across the boundary into the other grain. At the same time some vacancies condense in this high strain area to facilitate the transfer of atoms. This mechanism is schematically illustrated in fig.4. Support for the mechanism involving jumps of groups of

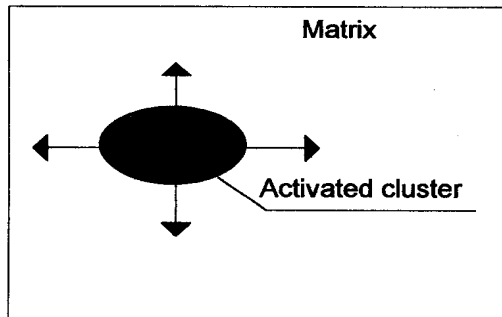


Fig. 3. Schematic representation of the activated cluster characterized by local temperature  $T_C$  and pressure  $P_C$ .

atoms is given in the paper of Wunderlich, this proceedings. On the other hand, for  $\langle 100 \rangle$  and  $\langle 111 \rangle$  boundaries, it is apparently possible that atoms jump from one crystal to the other individually or in small groups, taking the opportunity of a "hole" in the grain boundary structure formed by only one vacancy.

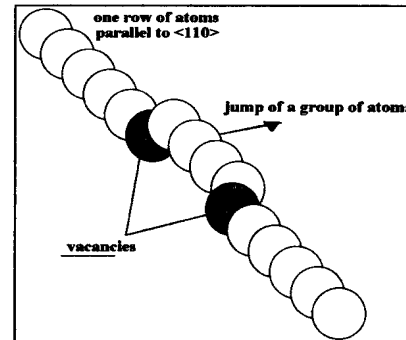


Fig. 4. Model of the mechanism of grain boundary migration by a jump of a segment of a  $\langle 110 \rangle$  dense packed row of atoms, with the participation of two vacancies.

#### CONCLUSIONS:

For  $\langle 110 \rangle$  tilt grain boundaries in Al grain boundary migration takes place by jump of close packed groups of atoms in a tightly packed space, so that the activated cluster is under a pressure reaching 4-5 GPa. The activation volume depends on misorientation and reaches 3 atomic volumes. For  $\langle 100 \rangle$  and  $\langle 111 \rangle$  tilt boundaries the activation volume is constant and close to one atomic volume.

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