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Mechanical Properties of Grain Boundaries and Triple Junctions in Metals

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Abstract. When a bicrystal or polycrystal are subjected to a change in temperature, the individual responses of the two adjoining crystals may differ in a manner which tends to produce a dilatational mismatch along grain boundaries. If compatibility is to be retained along the interface, an additional set of stresses must then be generated in order to conserve this compatibility. 'Compatibility stresses' will also be generated whenever a polycrystal is heated or cooled and the thermal expansion coefficients of the individual grains are different due to thermal expansion anisotropy . In such cases adjacent grains will attempt to change dimensions and develop mismatches by amounts controlled by the parameter $\Delta a^*\Delta T$, where Δa is the difference between the thermal expansion coefficients in the appropriate directions, and ΔT is the temperature change. These 'compatibility stresses' may be relieves if grain boundary motion, triple junction migration and grain growth are possible. These 'compatibility stresses' may play important role in the kinetic behavior of the microstructure ranging from influencing the behavior of lattice dislocations near the grain boundaries to promoting grain boundary and triple junction dragging or moving. The motion of grain boundaries, triple junctions and grain growth under the influence of internal mechanical stresses is the main subject of this paper.

Introduction.

Interfaces exert profound effects on the mechanical properties of bicrystals and polycrystals. These effects appear in a wide variety of forms and stem from a wide range of sources. Temperature plays a decisive role in determining many of the mechanical properties of grain boundaries and triple junctions. It has been recognized by many investigators that thermal expansion anisotropy is a potential source of microfracture during thermal excursions [1-4]. The incidence of microfracture in specific systems has been shown to depend on the scale of the microstructure [3] (the grain size, shape and misorientation in single phase materials).
We discuss material typified by the hexagonal crystal structures where the coefficient of thermal expansion in any direction of the basal plane is a_a and in the orthogonal direction a_c . The expansion coefficient a_ω at an arbitrary angle ω to the c-axis in a section normal to the basal plane is [5]

$$a_\omega = a_c \cos^2 \omega + a_a \sin^2 \omega = a_a + (a_c - a_a) \cos^2 \omega \qquad (1)$$

Consider two grains joined at a grain boundary . In general the c-axes of the two grains lie at arbitrary angles β and γ to the grain boundary. For simplicity we examine first the case when the c-axes lie in the grain boundary plane, i.e. $\beta = \gamma = 0$ [5]. The direction of the maximum strain

corresponds to the maximum separation of the ellipses at symmetrical positions defined by ω^* in [5]. The value of ω^* is found by maximising

$$|\Delta a| = [\, a_c \cos^2\omega + a_a \sin^2\omega\,] - [\, a_c \cos^2(\omega+\theta) + a_a \sin^2(\omega+\theta)\,[\cos^2\omega - \cos^2(\omega+\theta)] \quad (2)$$

Differentiating with respect to ω gives

$$\frac{d|\Delta a|}{d\omega} = (a_a - a_c)[\sin 2\omega - \sin 2(\omega+\theta)] \quad (3)$$

Equating to zero gives $\omega^* = (45-\theta/2)$, which locates $|\Delta a|_{max}$.
The variation of the relative magnitude of the maximum strain with θ is shown in [5].
For the general situation when the c-axes of the two grains are not in the grain plane the two ellipses representing the thermal expansion in the boundary plane are of different size. The minor axes are always equal to a_a and the major axes vary between a_a and a_c [5].
The difference in expansion coefficients in an arbitrary direction ω is now

$$|\Delta a| = (a_c - a_a) - [\cos^2\beta \cos^2\omega - a_a \cos^2\gamma \cos^2(\omega+\theta)] \quad (4)$$

Differentiating as before shows that $|\Delta a|_{max}$ occurs when

$$\frac{\sin 2\omega^*}{\sin 2(\omega^*+\theta)} = \frac{\cos^2\gamma}{\cos^2\beta} \quad (5)$$

The aim of the current paper is to develop some aspects of the problem in polycrystalline brittle materials to polycrystal hexagonal metals at the experimental level. The properties of metals are controlled intrinsic thermal properties in addition to the microstructural factors.

Experiment and Results

The material selected for study was a hexagonal zinc, where there is differential expansion between the a- and c-axes, stresses and strains are set up around grain boundaries . The maximum differential grain boundary strain ε_{max} is simply proportional to the maximum difference in expansion coefficients $|\Delta a|_{max}$ and the temperature difference (ΔT)

$$\varepsilon_{max} = |\Delta a_{max}| * \Delta T \quad (6)$$

The difference in expansion coefficient between the c and a axes of Zn $|\Delta a|_{max} = 4.6*10^{-5}\ C^{-1}$.

The stresses and strains around boundaries and triple junctions can :

1. Drive the grain boundary and triple junction .
2. Change the grain boundary and triple junction structure.
3. Create the conditions for strain induced recrystallization

The results in the paper represents three original experiments.

1. Motion of the individual planar grain boundary.
2. Motion of the same triple junctions in the opposite directions.
3. Grain growth in the polycrystal strips with fine grain size.

1.The study of the velocity planar grain boundary was carried out on zinc bicrystals (the direction[1120] is perpendicular to surface sample) with maximum angle misorientation (86 -90°) around direction [1120] . Bicrystal of Zn were grown by directional crystallisation technique, using high purity 99.995 at % zinc. The form of the grain boundary with the planar facets is shown on Fig.1. Samples were annealed at 350- 410 C° for various times, between 1 and 60 min to obtain

the motion of planar grain facets. The samples were examined *in-situ* in the optical microscope using reflected polarised light [6].

2. The study of the velocity triple junction motion was curried out on zinc tricrystals. Tricrystal of zinc were grown by directional crystallization technique, using high purity 99.995 at % zinc [7]. The scheme of the triple junctions moving in opposite directions are shown on Fig.2. Samples were annealed at 350- 410 C° for various times, between 1 and 60 min to obtain the motion of the triple junctions. The samples were examined *in-situ* in the optical microscope using reflected polarized light.

3.The study of the grain growth in polycrystal was curried out on zinc polycrystals strips with fine grain size (the initial mean grain size was 0.1mm) . Samples were annealed at 200- 410 C° for various times, between 1 and 60 min to obtain grain growth. The samples were examined *in-situ* in the optical microscope using reflected polarised light.

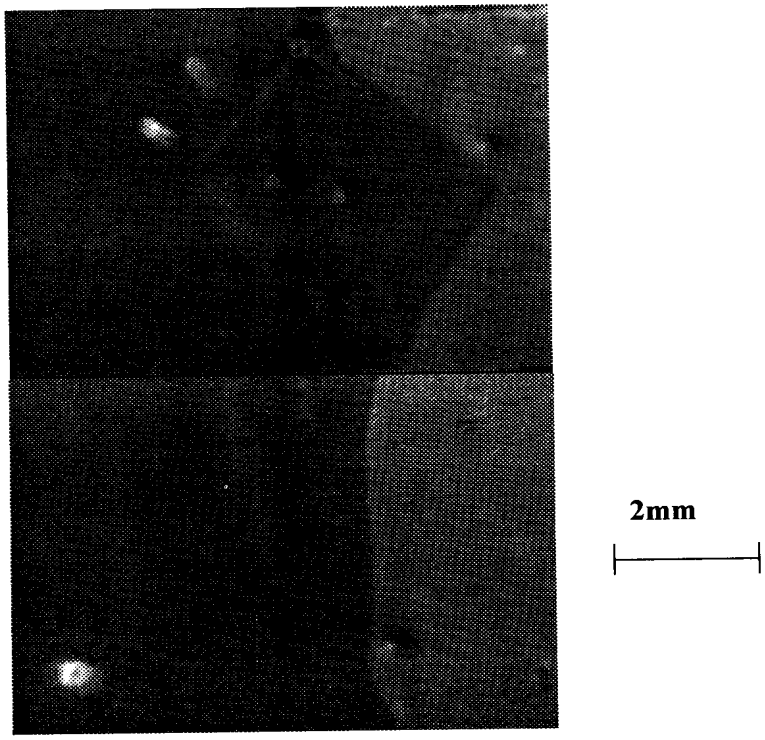

Fig.1. The view of zinc bicrystal with tilt grain boundary [1120] and planar facets.

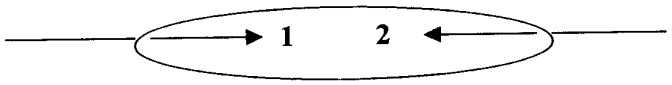

Fig.2. The scheme of the same triple junctions moving in opposite directions.

Results and Discussion

Fig.3 shows the Arrhenius plot of the velocity of planar facets. Apparently the stress driven facet is thermally activated process. We can determine the activation enthalpy for grain boundary facet motion from the slope of the Arrheniusline. The activation enthalpy for the motion of planar grain boundary facet is 1.08 eV and close to the activation enthalpy for the motion of curved [1120] tilt grain boundary in the same zinc [8].

Fig.4 shows the Arrhenius lines of the mobility of the same triple junctions in the opposite sites. Apparently the curved and stress driven triple junction are thermally activated process. We can determine the activation enthalpy for the triple junction motion from the slope of the Arrheniusline. It is shown that at relatively low temperature the motion of the triple junction (1) is determined by the triple junction mobility, while at elevated temperatures grain boundary mobility controls the migration of triple junction. The motion of the triple junction (2) is different. The motion is determined by triple junction mobility at all temperatures [9].

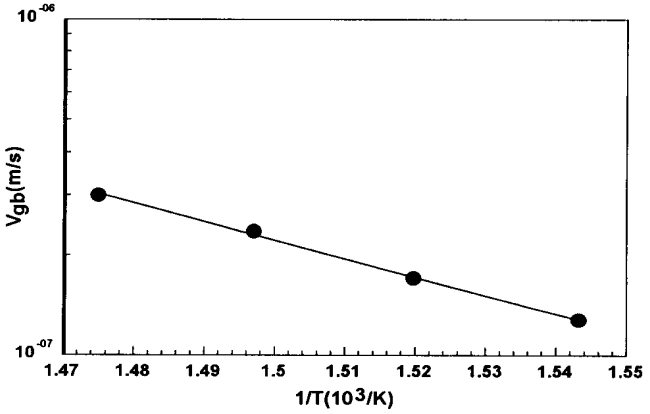

Fig.3. The temperature dependence of the grain boundary velocity in zinc bicrystal.

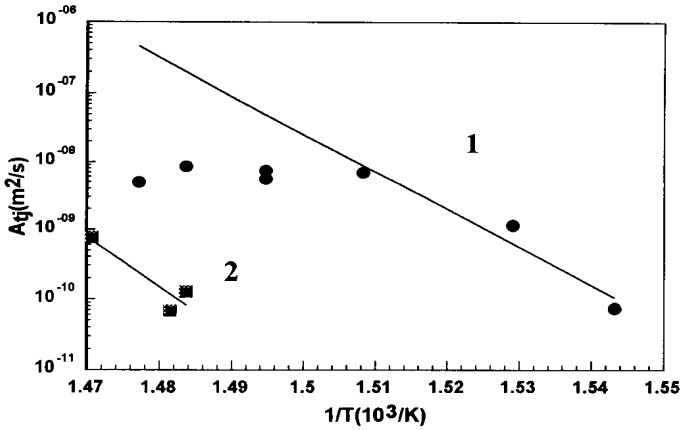

Fig.4. The temperature dependence of the triple junction mobility for the same triple junctions moving in opposite direction according Fig.2.

Fig.5 shows the temperature dependence of mean grain size in polycrystalline zinc strips. We observe the sharp increasing in mean grain size. The velocity of mean grain size sharp increases at $T=0.71T_{melting}K(200\ C^{\circ})$ and becomes $2.4*10^{-6}$m/s Fig.6.

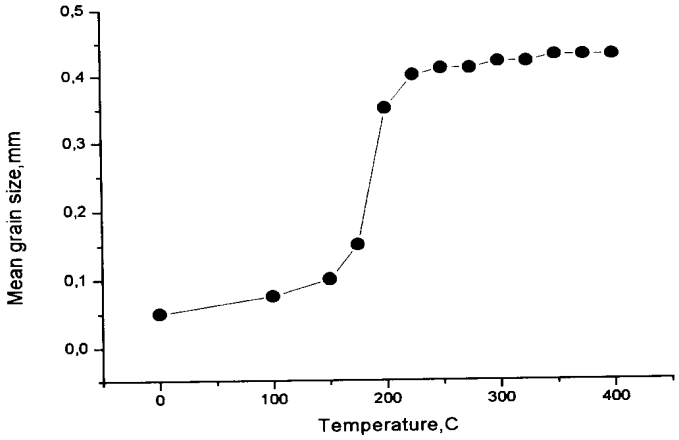

Fig.5.The temperature dependence of mean grain size in zinc polycrystal strips.

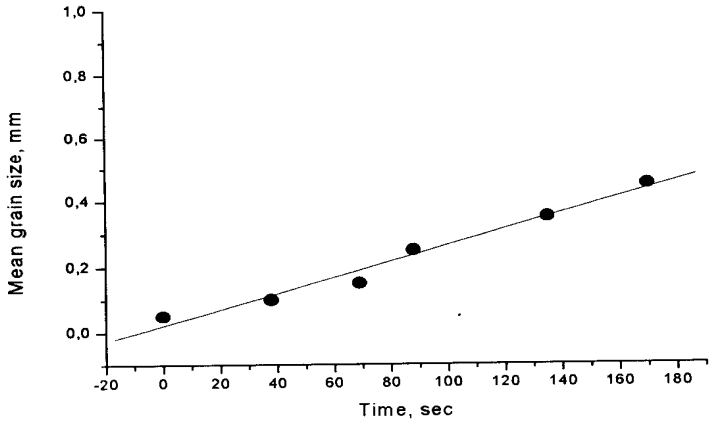

Fig.6. The time dependence of mean grain growth in zinc polycrystal strips.

Under thermal expansion anisotropy dislocations are formed and approach grain boundaries, then are submitted to forces which may or not may not help their motion towards and their impingement on these interfaces. There are two additional forces in the presence of an interface: the image force due to the long-range elastic interaction between the two defects and the force due to the interaction between the defect cores. The image forces occur for grain boundaries in anisotropic

materials. The image force intensity may be of the same order of magnitude as the other forces acting on the dislocation and must be taken into account in the "dislocation – interface" interaction. When lattice dislocations impinge on interfaces at low temperature, the interfaces play the role of strong obstacles for slip transfer. When the temperature increases, some lattice dislocations may enter the interfaces leading to the formation of extrinsic grain boundary dislocations. In order that other dislocations may penetrate again, the stresses associated with the extrinsic dislocations may be relieved. This may be realised in the neighbouring crystals by transmission, and occasionally by reflection. In these cases , the interfaces play their role of sources for lattice dislocations. The stress relaxation may also occur within the interface by two alternative processes: core delocalization or incorporation within the interface structure. In these cases, the interfaces play their role of sinks. Whatever be the relaxation mode, it strongly depends on the interface structure.

Until now we have considered the interaction between a dislocation and grain boundary in a bicrystal, i.e. a"free" grain boundary. In order to go towards polycrystals, we now have to consider a grain boundary which is constrained at triple junctions. Finally, stresses accumulated at triple junctions may accommodate by appearance the new grains or cavitation. The different grain boundaries are more or less active according to their structure and chemistry. Although atomic details control the relaxation at each interface, the contribution of all the interfaces to a macroscopic property must roughly depend on the grain boundary "caracter" distribution in the polycrystal. Not only the proportion of the different grain boundaries but their repartition in the polycrystal space has to be considered.

Summary

Experimental results shows the strong effect of the stresses and strains from thermal expansion anisotropy on kinetic properties of grain boundaries and triple junctions in zinc. The influence of anisotropy is the one of the main reasons of strain induced recristallization in zinc.

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