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Plasticity of grain boundaries*

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Plastic deformation of a polycrystalline body requires the propagation of slip bands from one grain to another. This process may occur by dislocations being forced through boundaries, new dislocations being nucleated in or adjacent to the grain boundary, or pinned dislocations being released. Whichever of these processes dominates, it is necessary for the grain boundary structure to be reshaped, and in previous work (Pond & Smith, 1977; Pond *et al.* 1977) we have described experimental observations of grain boundary dislocation processes involved in such activity.

It is well established that grain boundary embrittlement in metals is associated with segregation of impurity elements, although not all segregants result in brittle behaviour. It is argued here that the key effect of solutes is on the propagation of slip from one grain to another. In the absence of precipitation, segregation may be described as giving a very large hardening effect. The purpose of this paper is to discuss the distribution of solute at grain boundaries in such cases and based on the results of atomistic calculations of relaxed grain boundary structures in aluminium (Smith *et al.* 1976; Pond *et al.* 1978).

Periodic relaxed ⟨100⟩ and ⟨110⟩ tilt grain boundaries have been studied. The most significant result of this work is that minimum energy relaxed structures for given grain misorientations and boundary plane orientations are characterized by groups of atoms resembling those in liquid metals as described by Bernal (1964). A general trend was that grain boundary energy tended to decrease as the proportion of boundary material composed of such random close packed (r.c.p.) groups, as Bernal called them, increased. On the other hand, grain boundary energy was not related to the dimensions of the boundary period, for example, as suggested by the coincidence model of grain boundaries. The observation of r.c.p. material in low energy structures was so general that we suggest that even non-periodic boundaries in close packed metals tend to be composed as far as possible of r.c.p. material (Pond & Smith 1977).

In general, the crystals adjoining the boundary impose constraints that do not exist in liquids and as a consequence the relaxations that can occur and the groups that can be formed are restricted. Thus not all of the boundary material can be described in terms of r.c.p. groups, and other more complex polyhedral groups are formed. Analysis in terms of r.c.p. and complex polyhedra can be useful in understanding segregation. Since the polyhedra at boundaries may differ from those in the crystal interiors, they can provide favourable sites for both interstitial and substitutional segregants. Analysis of boundary structures is presented from two points of view: first, the relation between crystallographic parameters of boundaries and the distribution of r.c.p. and complex polyhedra, and secondly, the dimensions of segregants able to occupy substitutional and interstitial sites in r.c.p. and complex polyhedra are discussed.

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