22: Diffusion transport in polycrystals: the Nature and the significance of grain boundaries

Flow Chart

•Describe the geometrical relationship between the movement of atoms and strain

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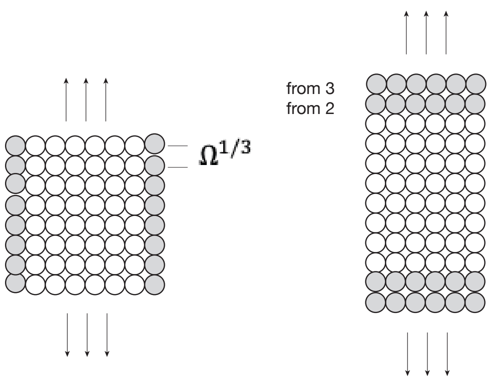

•Consider the rate of movement of atoms by diffusion

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•Describe the equations the prescribe the influence of applied stress to the diffusion flux

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•Obtain the equation for the strain rate in terms of the applied stress, the grain size and the temperature.

$$\dot{\varepsilon} = A\frac{\sigma^n}{d^p} D_O e^{-\frac{Q}{RT}}$$

The Role of Grain Boundaries

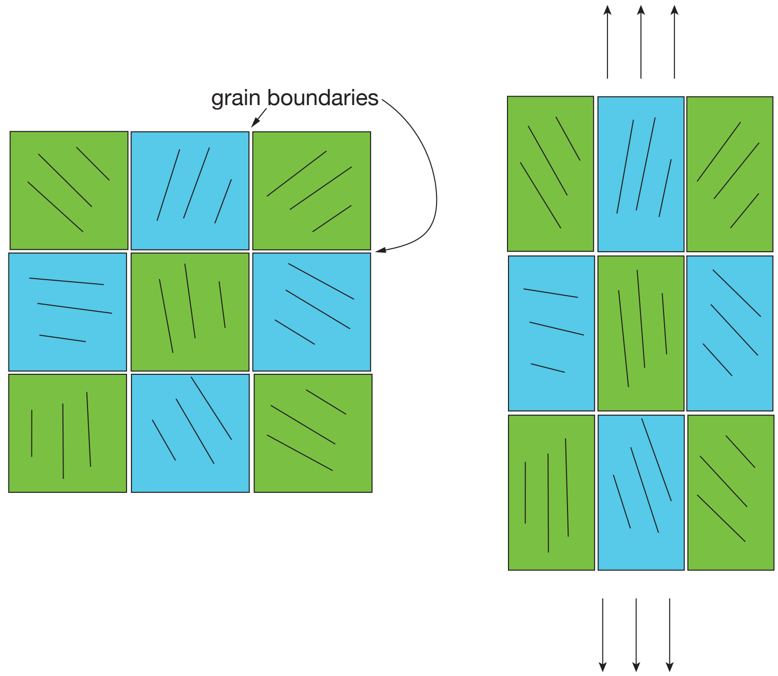
Deformation by Mass Transport in a Polycrystal

As shown in the schematic on the next page the mass is transported in the same way in a polycrstal as in a single crystal that is from one crystal face to another. Therefore the strain can be calculated in a unit problem, that of a cubic single crystal and applied directly to a polycrytals with the following caveates:

(i) In an open single crytal the atoms were etched and plated on the free surface of a single crystal

(ii) In a polcrystal they must be etched and plated at grain boundaries

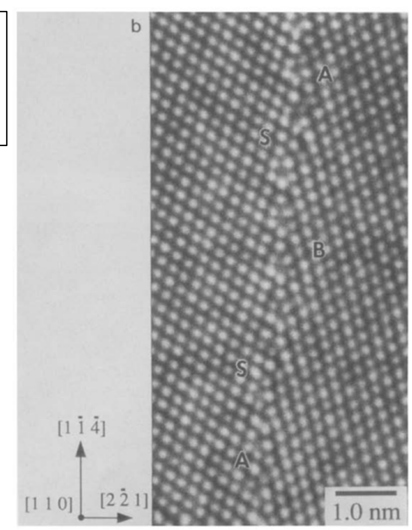
(iii) So the question arises what is the uniqueness of the atomic structure of grain boundareis that maked (ii) possible?



Question: What is the structure of the grain boundary that enables it to serve as a site for crytal growth when atoms are inserted into it, or recession when atoms are removed from the grain boundary. (Recall that the study of crystal growth from a melt like growing a single crystal of silicon from a metlt, or crystal growth from a vapor phase, like in molecular beam epitaxy is explained by the growth of ledges in the surface that creates corners where atoms from the melt or the vapor phase can stick). So we think that grain boundaries may also have such ledges where can be deposited or removed.

An electron micrograph (taken from a transmission electron microscope) of the grain boundary does indeed show the presence of ledges at a grain boundary,

Reference: "Mills MJ, Daw MS, Thomas GJ, Cosandey F. High-resolution transmission electron microscopy of grain boundaries in aluminum and correlation with atomistic calculations. Ultramicroscopy. 1992 Mar 1;40(3):247-57."



•A Grain boundary is an entity where to crystals that are misoriented with respect to each other come together.

•The crystals reach each other at atomic level until they touch without losing the coherence of thier instrinic structure, that is the structure of the two crystals is nearly perfectly maintained in the closest quarters of the grain boundary.

•The structure of the boundaries is characterized by steps and ledges just like in a single crystal with a free surface.

•The ledges can grow or etch to add atoms or remove atoms without undoing the coherence of the atomic structure of each crystal.

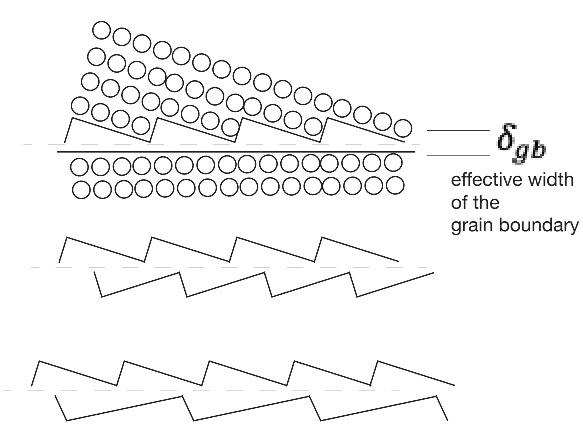
To show above with a schematic

•The schematic shows that the grain boundary as an effective width which is expected scale $\Omega^{1/3}$

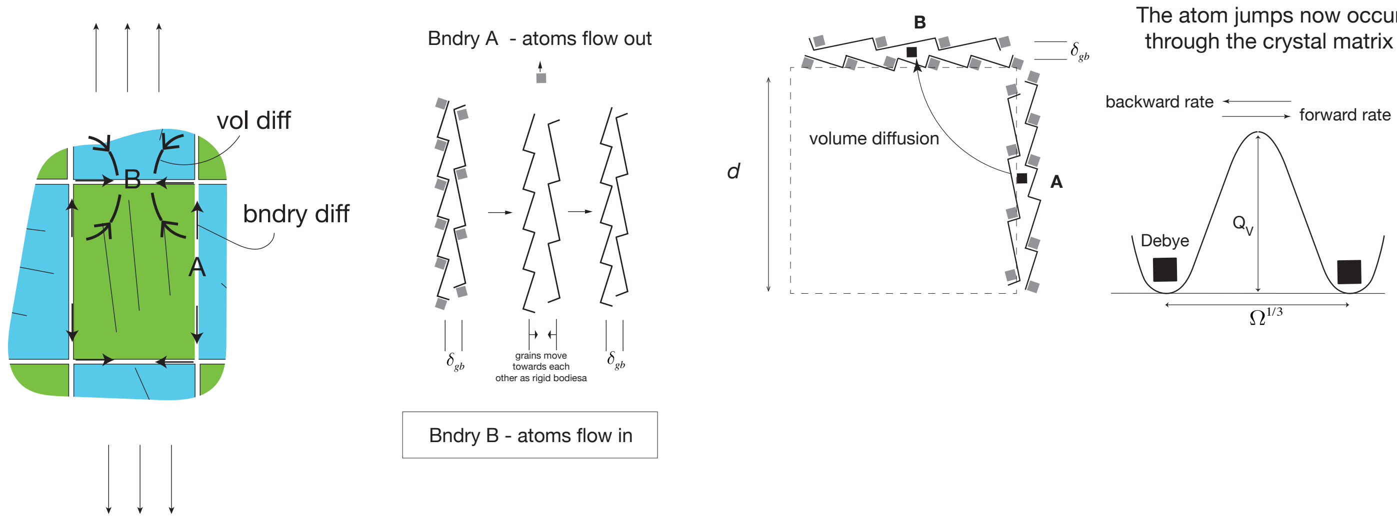
We write that

$$\delta_{gb} = 2.5\Omega^{1/3}$$

•The ledges can grow or recede as the atoms are added or removed from the grain boundaries.



Dffusion Transport by “Volume Diffision”
that is, by diffusion through the grain matrix crystal



•It is intuitively obvious that the transport of atoms from the side to the top is a product of two quantities: (i) The applied stress which provides the thermodyamic driving for the atoms to move from the side to the topp (just like the gradient of a slope provide the driving force for a ball to roll down the hill). This driving force is a gradient in energy. Note that the gradient of energy (force time displacement) is a force. (ii) I the rate at which atoms can be transported in the direction of the driving force. This transport mechanism is called diffusion.

•In the above schematic the atoms can diffuse along two pathways, along the boundary, and through the matrix of the crystal. These are called grain boundary diffusion and volume diffusion and are distinguished by the D_{gb} and D_V nomenclature.

• Note that these two pathways are additive that is both D_{gb} and D_V add together to provide the total rate of mass transport. The "rate" enters through the diffusion coefficient which has units of $m^2 s^{-1}$.

Next Sequence of Topics

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