04/13/2020

Lecture Notes from Monday 04/13/202

Hi-Temp

Topics

(i) Superplasticity: and example of high temperature deformation in ceramics.
(ii) Mechanism of deformation
(iii) Solid State Diffusion

Superplastic deformation in polycrystalline zirconia

See paper by Wakai et al. (1986), cited below:

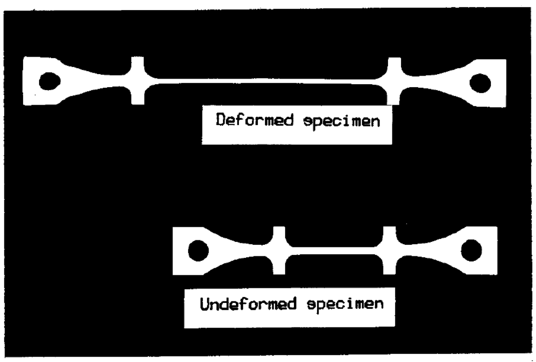


Fig. 1. Superplastically elongated specimen of Y-TZP at 1450°C.

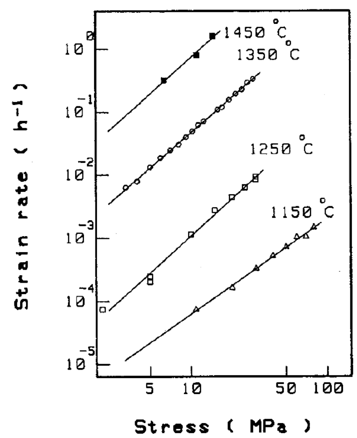


Fig. 3. Steady-state creep rate vs applied stress for Y-TZP.

cross-head speed of 0.05 to 1.0 mm/min. The elongation of the specimen was estimated by the displacement of the cross-head.

Notes: (i) large elongation without necking, strain rates as high as 1 h^{-1}, that is strain of 1 (engineering strain of 230%) in one hour.

Mechanism of Deformation

Notes:
(i) The shape of crystals can be changed by transporting atoms from one crystal face to another.
(ii) In a polycrystal all crystals can change their shape in this way so that the strain in one grain is also the strain in the whole polycrystal.
(iii) The role of grain boundaries?
(iv) Two pathways for diffusion.
(v) The vacancy mechanism for mass transport through the grain.
(vi) The form of the diffusion coefficient. ^{2}=6Dt

$$D = D_o e^{-\frac{Q}{RT}}$$

Approach

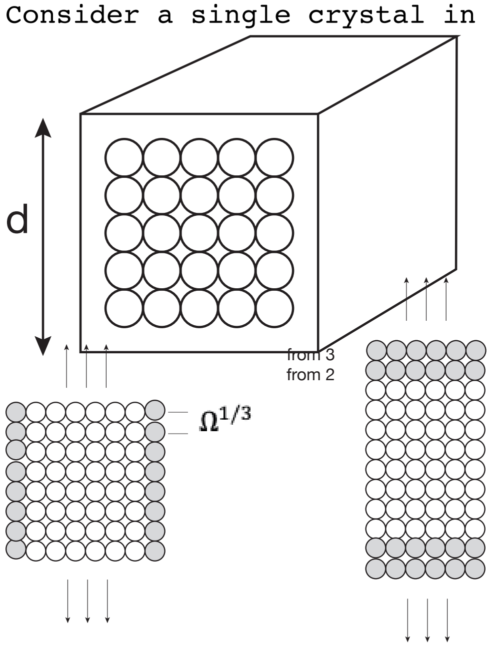
(i)Unit of mass transport, volume wise, Ω.
(ii)Calculate the strain from atom by atom transport of mass. Consider a stand also single crystal in the shape of a cube, with an edge length, *d*, which becomes the grain size in a polycrystal
(iii)How does the deformation of a single crystal pertain to the deformation of a polycrystal which is an aggregate of many “grains”. The interfaces between adjacent grains, called grain boundaries, have a special property: that atoms can be absorbed into interfaces, or depleted from the interfaces. Why, and how?
(i), (ii) and (iii) allow us to calculate the strain-rate in the polycrystal to the flux of mass transport. These issues are related to the geometry of mass transport- it is the mechanism of deformation.

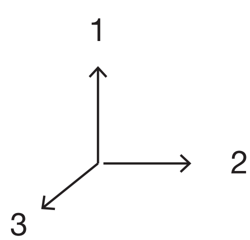
Next class of issues, is related to the mechanism of mass transport in the solid state (by diffusion) and also the driving force for mass transport induced by the applied stress.

Ultimately by combining the geometry of mechanism with the kinetics and the driving force for mass transport we can obtain an equation that related the strain rate, to the temperature, the applied stress and the microstructure (the grain size the grain boundary behavior).

Relationship between Transport of Atoms and Strain in a Single Crystal

Consider a single crystal in the shape of a cube:





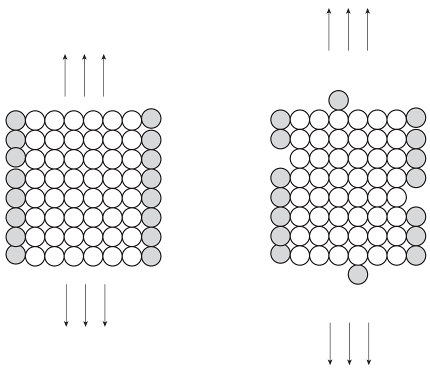
(Figure 1) Now we consider the etching of atoms from faces 2 and 3, and depositing those atoms on face 1, as shown below.

(Figure 2) We shall use **Ω as the volume** occupied by one atom. Therefore the size of the atom is given by $\Omega^{1/3}$ and the area occupied by the atom on the surface is given by $\Omega^{2/3}$.
In the above figure atom layers from face 2 and face 3, from both sides of the crystal are etched and plated on to face 1, as shown on the right.

The strain along “1” is then given by

$$\varepsilon_1 = \frac{4\Omega^{1/3}}{d} \qquad (1)$$

While the transverse strains are negative and equal to one half of the axial strain so that the sum of the principal strains is zero (the constant volume condition), that is $\varepsilon_2 = \varepsilon_3 = -\frac{1}{2}\varepsilon_1$.
Now we wish to consider if only one or two atoms are etched and moved to the “1” face, as shown below



(Figure 3) In this instance we move two atoms (total) from the transverse faces to the face to which we have applied a tensile stress. The tensile strain will now be given by Eq. (1) but weighted by a factor that is equal to two atoms divided by the total number of atoms moved in Figure 2. This weighting factor is equal to

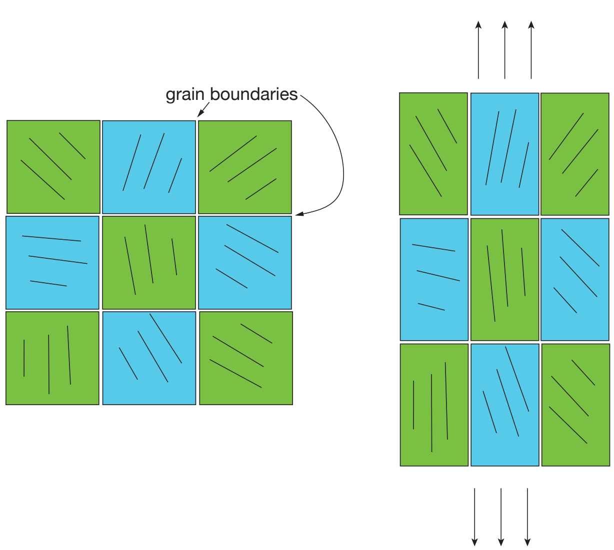
$$weighting\ factor = \frac{2}{\#atoms\ moved\ in\ Fig\ 2} = \frac{2}{4\frac{d^2}{\Omega^{2/3}}} \quad (2)$$

The denominator in Eq. (2) has the factor 4 represents the four layers that were plated on the “1” face, while the factor $\frac{d^2}{\Omega^{2/3}}$ is equal to the number of atoms present in the full layer over the surface area of the crystal which is equal to d^2. Multiplying the right hand side of Eq. (1) by Eq. (2), the weighting factor we obtain the result for the strain arising from moving just the two atoms,

$$\varepsilon_1 = \frac{4\Omega^{1/3}}{d}\frac{2}{4\frac{d^2}{\Omega^{2/3}}} = \frac{2\Omega}{d^3} = \frac{2\Omega}{d^2}\frac{1}{d} \quad (3)$$

Note that Eq. (3) can be interpreted generally as follows: the thickness of the layers deposited on the transverse face is equal to the volume of the material deposited (2Ω), divided by the area on which it is deposited, d^2, as given by the first term on the right hand side. The strain is then equal to the thickness of this layer divided by the grain size, as given by the second term.
In summary it is possible to obtain strain by transporting atoms from side faced to the face to which a tensile stress has been applied.

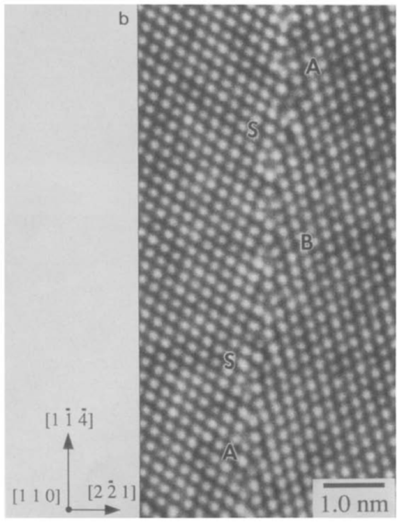
Relating the Single Crystal Mechanism to a Polycrystal



(Figure 4) The figure on the left shows the deformation of a polycrystal. Each crystal deforms in the manner discussed in the previous section, but in a way that is compatible with other crystals surrounding it.
The subtle point about the above scenario is that grain boundaries can serve as the source and the sink for atoms, just like the free surfaces in the previous discussion. Thus we are impelled to consider what is the *structure of the grain boundaries* that makes that possible. Recent work by high resolution transmission electron microscopy has

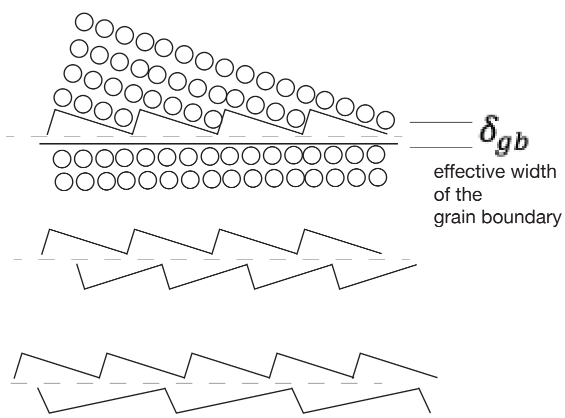
shown that the lattice planes of the adjacent crystals extend up to the grain boundary plane as shown in the atomic scale resolution micrograph of a grain boundary in aluminum,

The Importance of Ledges in Grain Boundaries



(Figure 5) 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."

Note the presence of ledges in the boundary. Atoms can be added or removed from these ledges to make the crystal grow (along the axial direction) and recede (in the transverse direction) producing mechanical strain. The following schematics show different structures of the grain boundary arising from different degrees of misorientation between the adjacent crystals, and also orientation of the plane of the grain boundary.



(Figure 6) Notes: (i) Any misorientation between the crystals will necessarily give rise to ledges as the boundary. (ii) The ledges may be further apart or closer in as contrasted in the bottom two drawings. (iii) In the top picture one crystal is shown to be flat. However, a change in the plane of the boundary can introduce ledges in the bottom crystal.
In summary, misorientation between the adjacent crystals will produce ledges at grain boundaries.

Etching and Plating of Atoms at Ledges Leads to Strain (at constant volume)

The schematics on the left (on the next page in Fig. 7) show how atoms can be etched from the ledges (they are then plated on the adjacent grain boundary).

The adjacent crystals move closer to each other if the atoms are etched away, and further apart if atoms are inserted into the grain boundary. In this way the transport of atoms can produce strain as explained in the first example.

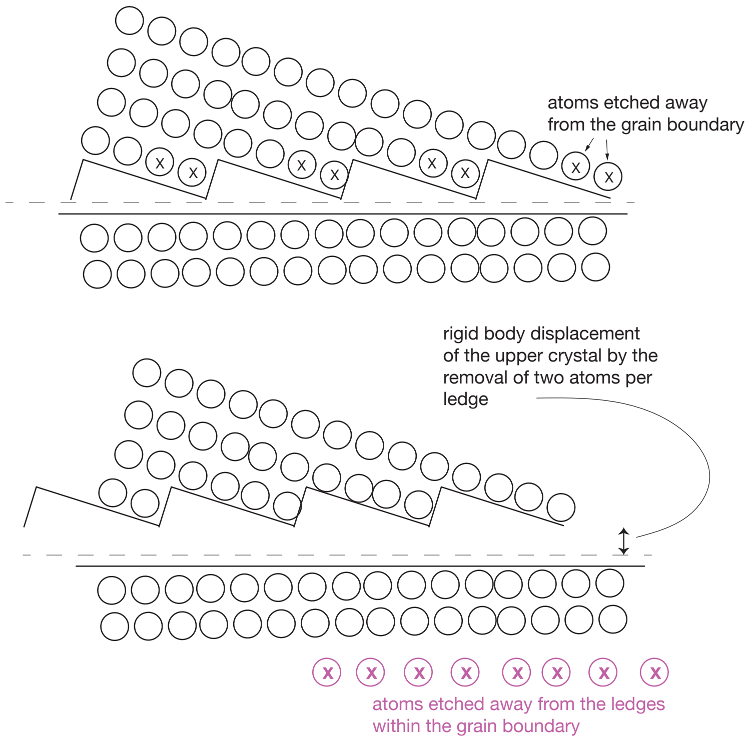


Figure 7:
Etching of atoms out of the boundary at ledge sites. As a result the two crystal move closer together as rigid bodies.

Relationship between Volume of Inserted Atoms and Strain

Earlier we had derived the strain from single atoms moving from the transverse face to the horizontal face.

Regardless of the structure of the boundary, the thickness of the layer deposited in a boundary (or conversely etched from it) will be equal to

$$\text{Thickness of the Deposited Layer} = \frac{toal\ volume\ of\ the\ atoms\ transported\ into\ the\ boundary}{surface\ area\ of\ the\ crystalite,\ which\ is\ equal\ to\ d^2}$$

Therefore the strain produced by the transport will be equal to the thickness, expressed above, divided by the grain size.

The above axiom holds for single atoms (as in Eq. 3), or for many atoms.

Practice Problems:

A polycrystal is assumed to be constructed from simple cubes. Each cube contains 10^6 atoms, that is its volume is this many atoms multiplied by Ω. The crystal is pulled in uniaxial tension. Calculate the strain that would be produced by the transport of 1000 atoms from every vertical grain boundary into the adjacent horizontal grain boundary.

Now assume that the atoms are transported at the rate of 1000 atoms per second. What will be the strain rate of the deformation of the polycrystal.