21: High Temperature: Geometry of mass transport

Key Features

•At high or elevated temperatures metals such that the strain increases with time

•Therefore the mechanical behavior is described by strain-rate

•The other parameters are the temperature and the applied stress, so that the behavior is described by the following functional form:

$$\dot{\varepsilon} = \frac{d\varepsilon}{dt} = f(\sigma, d, D)$$

where D is the coefficient of solid-state diffusion, σ is the stress, and d is the grain size.

Ω is the volume per atom in the crystal were the atoms are assumed to packed like small cubes.

$\Omega = \frac{\text{Mol wt}}{\text{density}}\frac{1}{N_A}$; therefore the distance between atoms $= \Omega^{1/3}$, and the area occupied by one atoms on a surface, for example is $= \Omega^{2/3}$.

Diffusion

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

There are two kinds of diffusion

Through the crystal (volume diffusion) $D_V = D_{OV} e^{-\frac{Q_V}{RT}}$

And through the grain boundary written as $D_B = D_{OB} e^{-\frac{Q_B}{RT}}$

•Diffusion has units of m^2s^{-1}, which are also the units for the pre-exponential, D_O .

•Q is called the activation energy - it is the energy barrier for atoms to move (or jump into) the adjacent lattice site.

•$\frac{Q}{RT}$ is dimensionless. Q had unit of kJ mol^{-1}, R =8.31 is the gas constant, J $mol^{-1}K^{-1}$, and T is K.

The range of values for Q are from about 50 to 300 kJ mol^{-1}.

Phenomenology of temperature dependent strain rate

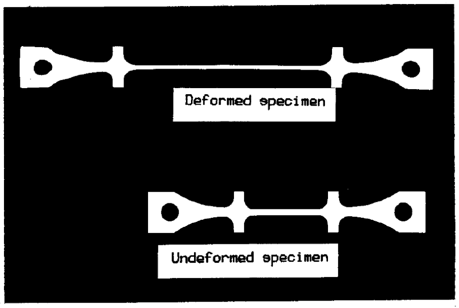

Fig. 1. Superplastically elongated specimen of Y-TZP at 1450°C.

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.

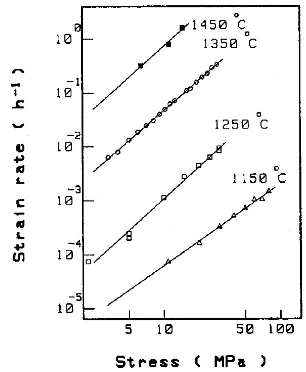

Fig. 3. Steady-state creep rate vs applied stress for Y-TZP.

Notes:

(1) Zirconium oxide is a brittle material, yet can deform to large strains at high temperatures (1150 °C to 1450 °C)

(ii) Phenomenological Description

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

$$\log_{10}\dot{\varepsilon} = \log_{10} A + n\log_{10}\sigma + \log_{10} D_O - \frac{Q}{2.3RT} - p\log_{10} d$$

Strain rate has units of s^{-1}, its magnitude can range from 10^{-10} per second (as in turbine blades) to $10^{-3}s^{-1}$ as in superplastic deformation.

Turbine blade is 0.10 m, let us say it has to last for 1000 h. How much stretch can be tolerate in this time.. Displacement of the tip must be less than 0.1mm

L	0.1 m	
DelL	0.1 mm	
	0.0001 m	
Strain	0.001	0.10%
time	1000 h	
	3.60E+06 s	
Strain rate	2.78E-10 per second	

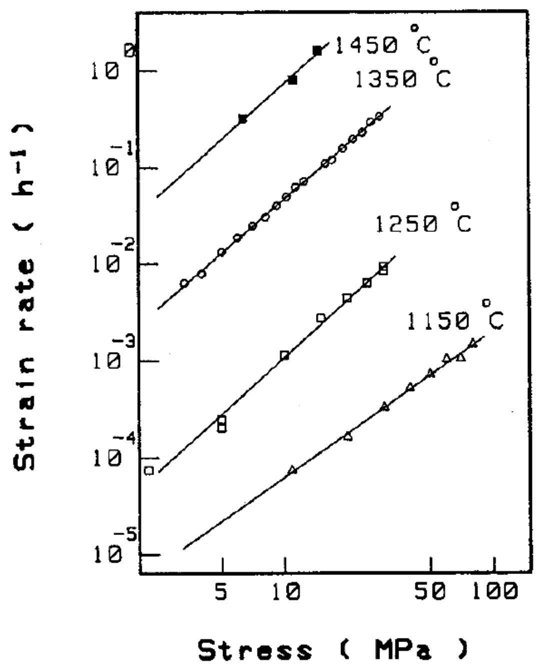

Fig. 3. Steady-state creep rate vs applied stress for Y-TZP.

How to analyze the data to obtain the parameters in the phenomenological equation (Practice HW 1)

Flow Chart

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

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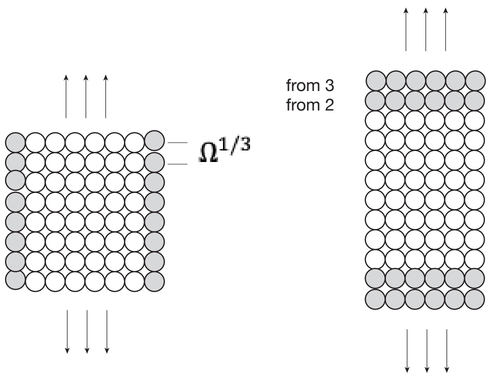

•Consider the rate of movement of atoms by diffusion

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

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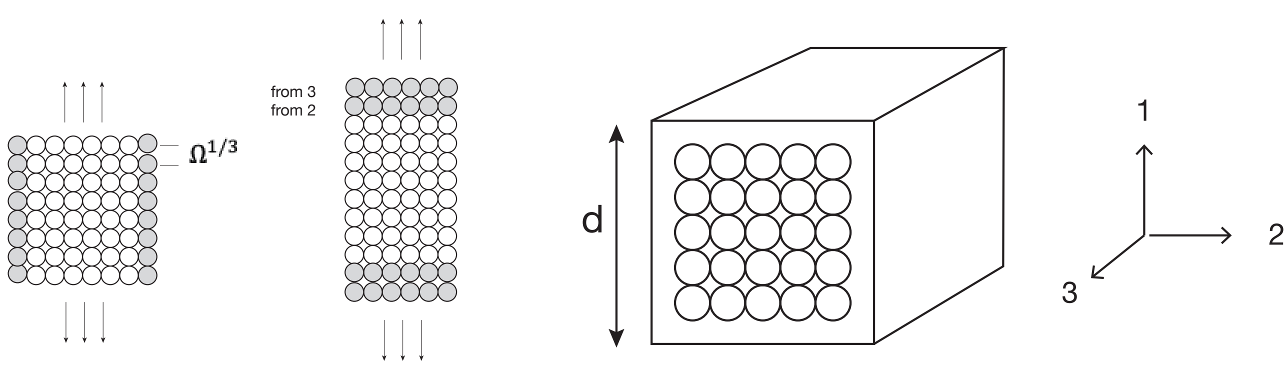
•Obtain the equation for the strain rate in terms of the applied stress, the grain size and the temperature.

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

The geometry of strain and atom movement in a small single crystal



The crystal is extending in direction 1 and shrinking in direction 2.

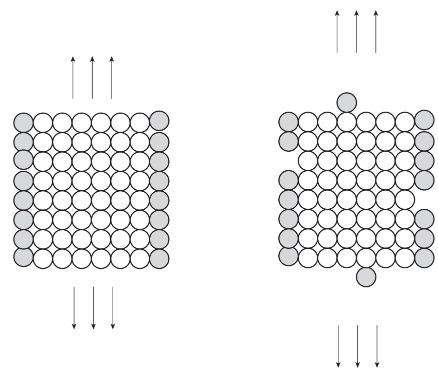
The volume must remain constant. Therefore the transverse strain in one half (and negative of the longitudinal strain)

$\dot{\varepsilon}_2 = \dot{\varepsilon}_3 = -\frac{1}{2}\dot{\varepsilon}_1$ the volume strain is the sum of the three and hence is equal to zero.

Area occupied by one atom on the surface = $\Omega^{2/3}$ thinking of the atom as occuping one cube of edge $\Omega^{1/3}$.

Let us not consider how much strain in direction one will be obtained if just one atom is moved from the side faces to the top and bottom faces.

So the growth of the top face (and the bottom face) by adding one atom to each face as shown will be given by



Average growth of each face

$$\frac{\text{the size of one atom*2(two faces)}}{\text{(size of the crystal)}} x \frac{\text{one atom}}{\text{total number of atoms on the face}}$$

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

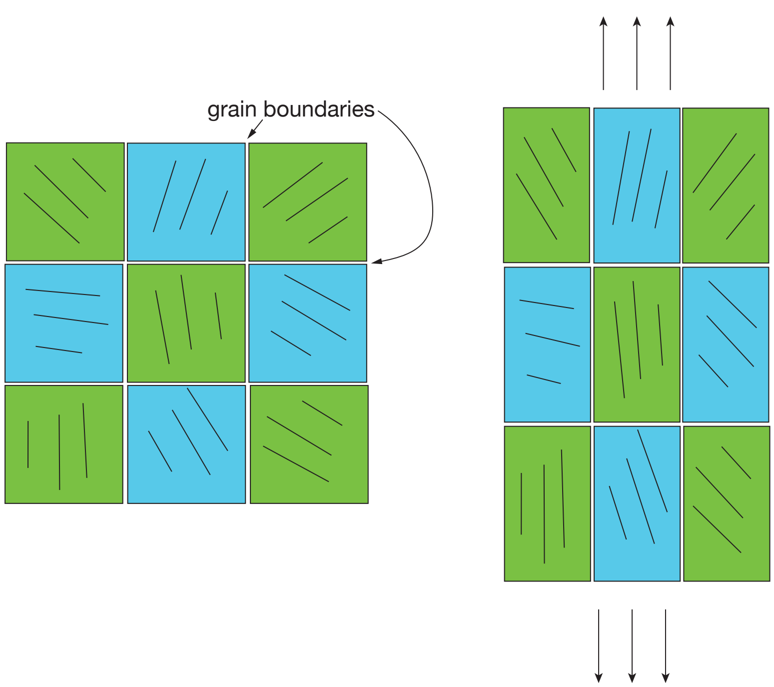
Let us say the flux of atoms being transported per unit time by diffusion is

J(number of atoms per unit area per unit time)x(area into which they are flowing=d^2)

Strain rate = strain per atom x #atoms per unit time

$\dot{\varepsilon}_1 = \dot{\varepsilon} = \frac{2\Omega}{d^3}Jd^2 = J\frac{2\Omega}{d}$ Units for the right side (atoms $m^{-2}s^{-1}*m^3m^{-1}$)= s^{-1} which is the strain rate.

Deformation by Mass Transport in a Polycrystal



Here mass is transported in the same way as in the case of a polycrystal that is, there is a source and a sink for atoms, but a fundamental question arises about how grain boundaries can serve in this capacity (source sand sinks)?