Bridging Length Scales

24: Chemical Potential and Atom Flux

Flow Chart

•Describe the geometrical relationship between the movement of atoms and strain (Lect 22)

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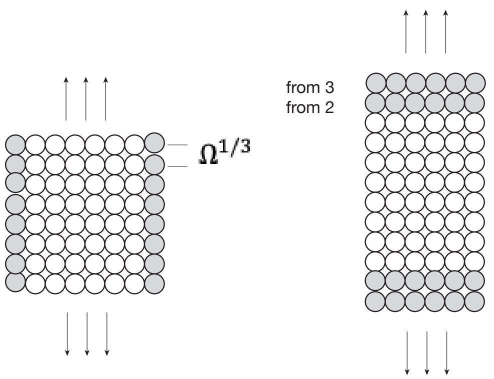

•Consider the rate of movement of atoms by diffusion (Lect 23)

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

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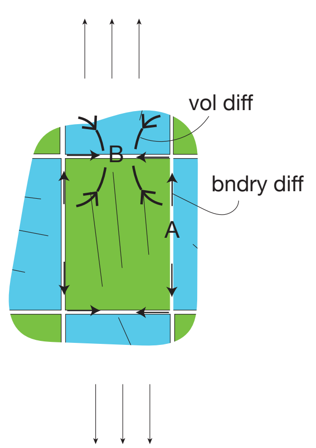
•Obtain the equation for the strain rate in terms of the applied stress, the grain size and the temperature. (Wednesday)

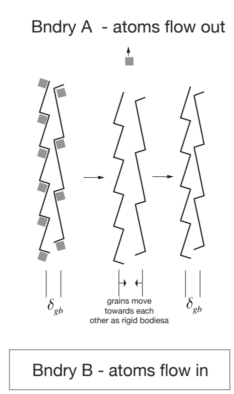
Notes:

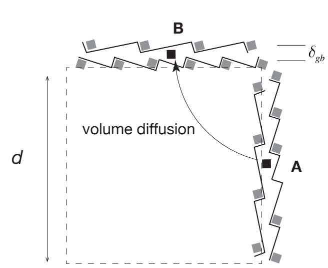
•There are two mechanisms for diffusional transport: lattice or volume diffusion, and boundary diffusion

•They contribute additively to the diffusion flux.

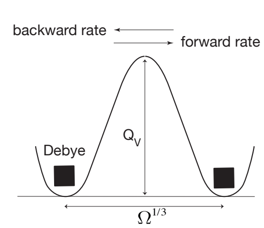
Dffusion Transport by “Volume Diffision”
that is, by diffusion through the grain matrix crystal

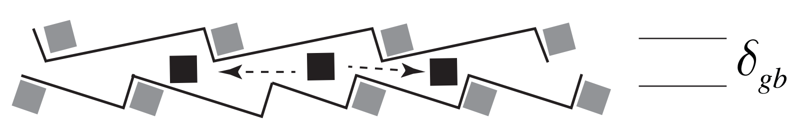






The atom jumps now occur
through the crystal matrix





Where we wish to arrive:

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

σ is the uniaxial stress

d is the grain size

D_O is the pre-exponential for the diffusion coefficient

Q is the activation energy for overcoming the energy barrier for atom jumps.

The Equation for Diffusion Flux

$$J = \frac{D_V}{\Omega k_B T}(\text{Driving Force})$$

The units for the driving $\frac{\text{energy (J)}}{\text{distance (m)}}$ (has units of force)

Driving force is a gradient of energy. And in Materials science we write the energy state **as a chemical potential with a symbol μ. Mu has units of energy or potential. Nearly always we are concerned not with the absolute value of mu but gradient of its values because the driving force for a physical phenomenon is related to what happens as a result of potential gradient.**

Therefore we write the driving force in a simple way as follows

$$\text{driving force} = \frac{\mu_1 - \mu_2}{\Delta x}$$

Where Δx is the physical distance from state 1 and state 2.

Units

The driving force has units of J/m

D_V has units of m^2s^{-1}

Omega m^3

k_BT thermal energy per atom J $atom^{-1}$

Right hand side has the following units

$$\frac{J(oules)}{m}\frac{m^2}{s}\frac{1}{m^3}\frac{atom}{J(oules)} = \frac{atom}{m^2 s^{-1}}$$

Therefore the left hand side, called the atom flux has units of atoms flowing through a unit cross section per unit time.

$$J = \frac{D_V}{\Omega k_B T}(\text{Driving Force})$$

The physical significance of the chemical potential

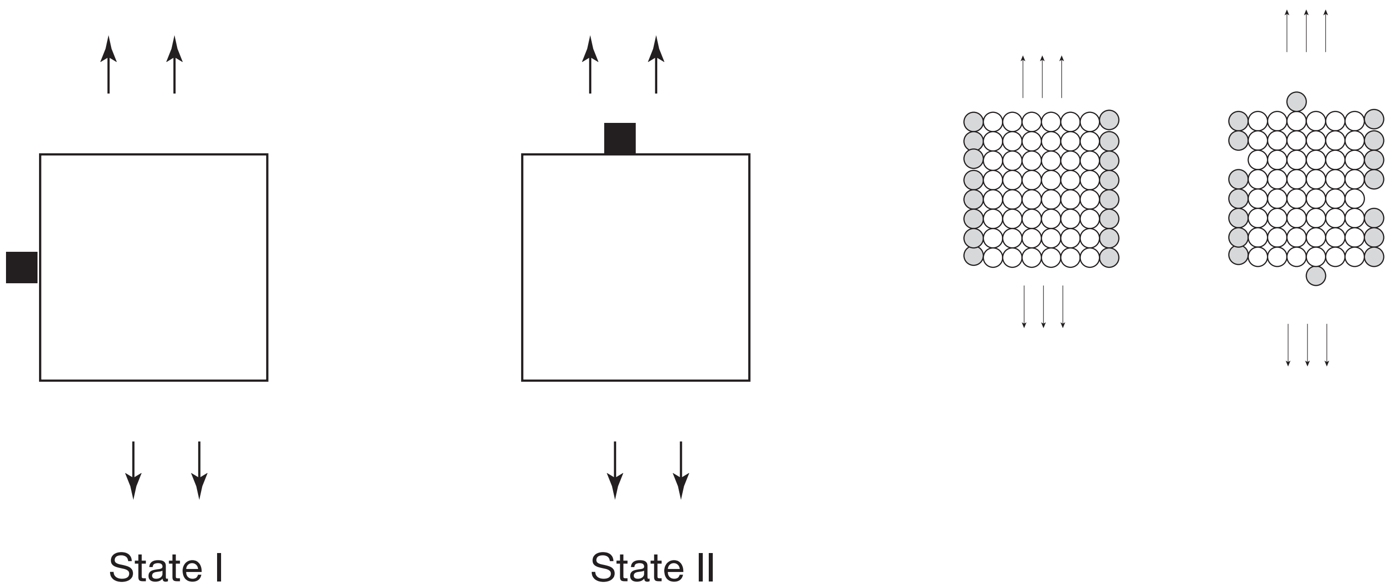
•The chemical potential is a state of energy that determines if work will be done by the surroundings on the system (in which case the chemical potential will increase), or the work is done by the system on the surroundings in which the chemical potential decreases.

•So we consider two states and the difference between the chemical potential of these two states. If State II has a lower chemical potential then I have a driving force for the atoms to migrate from State I to State II.

•Therefore the driving force is the difference between the start and the end state divided by the physical distance between those two states.

THE CHEMICAL POTENTIAL REFERS TO A GIVEN SPECIES. For example consider chemical potential of water. Say I have water and ice in contact and then I ask if the water will convert into ice or vice versa. The then from chemical potential point of view we ask if H_2O (the species) has a lower or higher chemical potential (here the chemical potential of water in these two states depends on temperature).

Stress Induced Chemical Potential



Here the species is the atom that is diffusing. The chemical potential in State II in lower than the chemical potential in State I, which divided by the distance gives the driving force/

$$\Delta\mu = \mu_I - \mu_{II} = \sigma\Omega$$

work done by the surroundings on the system = (force on the atom) x (displacement of the force)

=(foot print of the atom x stress)x (the height of the atom)

$$= (\sigma\Omega^{2/3}).(\Omega^{1/3}) = \sigma\Omega$$

To get the driving force I must divide $\Delta\mu$ by the distance of diffusion

$$J = \frac{D_V}{\Omega k_B T}(\text{Driving Force}) = \frac{D_V}{\Omega k_B T}\frac{\Delta\mu}{(d/2)} = \frac{D_V}{\Omega k_B T}\frac{2\sigma\Omega}{d}$$

$$J = \frac{D_V}{\Omega k_B T}\frac{2\sigma\Omega}{d} \qquad \text{m}^2\text{s}^{-1} \qquad (*)$$