

Chapter 1

Background and Some Concepts

Introduction

We assume knowledge of general solid state physics as in Rosenberg (1992). However, we shall begin by briefly summarizing a few concepts* that are basic to an understanding of later chapters below.

1.1. *Elastic and Plastic Regimes*

It is helpful to classify the discussion of mechanical properties by defining two regimes (i) elastic and (ii) plastic.

1.1.1. *Elastic Deformation*

The mechanical properties of materials are of vital importance in determining their fabrication and practical applications. Initially as a load is applied on the material, the nominal stress is defined as the load divided by the original cross section area, and the nominal strain as the extension divided by the original length. As the stress is increased, the strain increases uniformly and the deformation produced is completely reversible. This is so-called the elastic region. The stress and resulting strain are proportional to one another and obey Hooke's law.

From an atomistic point of view, if we pull two atoms apart or push them together by a force, the atoms can find a new equilibrium position in which the atomic and applied forces are balanced. The force in the bond is a function of the displacement. The deformation of the bond being reversible means that, when the displacement returns to the initial value, so does the force return

*Readers may skip this Chapter if they are familiar with this background material.

simultaneously to its corresponding value. The bulk elastic behaviour of large solid bodies is the aggregate effect of the individual deformations of the bonds which are the building blocks.

When the applied forces are sufficiently small, the elastic displacement is always proportional to force. This is Hooke's law. The elastic constant is a key parameter, to express the coefficient of proportionality between force and displacement. When the applied forces are large, the elastic displacement deviates from Hooke's law. The relation between force and displacement is nonlinear. This is then called nonlinear elasticity.

1.1.2. Atomic Forces and Elastic Properties

Taking NaCl type ionic crystals as an example, Cottrell (1964a) discussed the interaction energy of a pair of univalent ions at a distance r as

$$U(r) = \pm \frac{e^2}{r} + \frac{B}{r^s} \quad (1.1.1)$$

where, $s \approx 9$, and where + and - refer to like and unlike ions respectively. Having summed the repulsive and attractive interactions with nearest neighbours, the total interaction energy of an ion can be written as

$$U_z = -A \frac{e^2}{r} + 6 \frac{B}{r^s} \quad (1.1.2)$$

where A is called the Madelung constant, equal to 1.7476 for the NaCl type crystals. At the equilibrium condition, $\frac{dU_z}{dr} = 0$, at $r = r_0$. Thus,

$$B = \frac{Ae^2 r_0^{s-1}}{6s} \quad (1.1.3)$$

and

$$U_z = -\frac{Ae^2}{r} \left[1 - \left(\frac{1}{s} \right) \left(\frac{r_0}{r} \right)^{s-1} \right]. \quad (1.1.4)$$

This is the work required to dissociate the crystal into $2N$ separate ions (N positive and N negative).

The elastic constant E ,

$$E = \frac{f}{u} = \left(\frac{1}{6} \right) \left(\frac{\partial^2 U_z}{\partial r^2} \right)_{r=r_0} = \frac{(s-1)Ae^2}{6r_0^3} \quad (1.1.5)$$

where $\frac{U_z}{6}$ is the energy per each nearest-neighbour bond, and $u = r - r_0$, is the elastic displacement.

The bulk modulus of elasticity of the material is defined by

$$p = -K \frac{\Delta V}{V} \quad (1.1.6)$$

where p is a hydrostatic pressure, $\frac{\Delta V}{V}$ is the volume change.

$$K = \frac{-p}{\left(\frac{\Delta V}{V}\right)} = -\frac{pr_0^2}{r_0^2\left(\frac{\Delta V}{V}\right)} \cong \frac{f}{r_0^2\left(\frac{3u}{r_0}\right)} = \frac{1}{3r_0} \left(\frac{f}{u}\right) = \frac{(s-1)Ae^2}{18r_0^4}. \quad (1.1.7)$$

In KCl, it gives $K^T = 1.88 \times 10^{11}$ dyn cm², whereas the observed value (extrapolated to OK) is 2×10^{11} dyn cm². The corresponding calculations of elastic constants of metallic crystals are much more difficult for the laws of force are much more complicated. We shall discuss this in Chap. 5.

1.1.3. Plastic Deformation

Plastic deformation is characterized by a permanent deformation of the material. Unlike elastic deformation, it does not reverse on unloading but leaves the material with a permanent shape. This is called the plastic region. Between these two regions, there is a limiting stress, called the yield stress of the material, or the critical resolved shear stress for a single crystal.

The crystallinity of the structure is the prime cause of this behaviour, for it enables whole slabs of crystal to glide past one another. Each slip is a displacement, in certain glide direction, generally the crystal direction of closest atomic packing on certain crystal planes which is called the slip plane. In fcc and hcp metals, these are mainly close-packed planes, but in bcc metals, the situation is complicated. It will be discussed later. Slip begins on some small area of the surface.* The slip-front line between the slipped and unslipped areas is by definition a *dislocation* line. The glide motion of a dislocation is a property of a periodic crystal. The transition from the slipped to the unslipped region is spread over several atomic distances which is the width of the dislocation. Every atom in this transition region is pushed only a little further out of its original equilibrium site when it moves forward. This is the reason why dislocations can move easily in the crystal. Thus, the yield stress is much lower than the theoretical strength of crystals. Dislocation theory plays important role in understanding the microscopic processes in plastic deformation. Even the elastic theory of dislocations may explain many phenomena, such as yielding,

*See, for instance, the early paper of Chen and Pond (1952).

work hardening, etc. etc. It provides not only a deeper qualitative physical picture of plastic deformation but also to a certain degree a quantitative analysis of it.

Plastic deformation can also occur by twinning. The atoms slide, layer by layer to bring each deformed slab into mirror-image lattice orientation relative to the undeformed material. The critical stress of twinning is usually higher. Twins form at low temperature and under rapid deformation, e.g. bcc iron strained quickly at room temperature and slowly at 100K.

1.2. Griffith Criterion: Role of Surfaces

Griffith (1924) derived an expression for the elastic crack propagation on the basis of thermodynamic considerations. He reasoned that a crack would advance when the incremental release of stored elastic strain energy dW_E in a body became greater than the incremental increase of surface energy dW_s as new crack surface was created. For the two-dimensional case in plane stress

$$W_E = \frac{\pi\sigma^2 c^2}{E} \quad (1.2.1)$$

$$W_s = 4c\gamma_s$$

where, σ is the nominal stress; E , the elastic modulus; $2c$, the length of the crack, and γ_s the specific surface energy.

The Griffith criterion can then be written as with σ_F , the fracture stress,

$$\sigma_F = \sqrt{\frac{2E\gamma_s}{\pi c}} \quad (1.2.2)$$

by the condition that

$$\frac{\partial}{\partial c} W_E \geq \frac{\partial W_s}{\partial c}.$$

Subsequent analysis* in fracture mechanics defines a parameter, crack extension force, $G = K^2/E$ (in plane strain) being equal to a critical value, G_{Ic} ,

*This is associated with the names of Irwin (1957) and Inglis (1913). The analysis given by Inglis has been generalized by R. Lofstedt (Phys. Rev. *E55*, 6726, 1997) who has proposed an inequality involving a ratio of time scales to determine whether a material is brittle or ductile. One time scale is 'ductile', and is associated with the rate of decrease of the tensile stress at the tip of a narrow crack. The above ductile time scale is to be compared with a characteristic 'phonon time' a/v_s , where v_s is the velocity of sound, and a measures the lattice spacing. See also R. W. Armstrong (Mat. Sci. Eng. *1*, 251, 1996) also A. Kelly, W. R. Tyson and A. H. Cottrell, Phil. Mag. *15*, 567, 1967 and J. R. Rice and R. Thomson, Phil. Mag. *29*, 73, 1974).