2B_Upper Bound of Strength in Ceramics

Summary

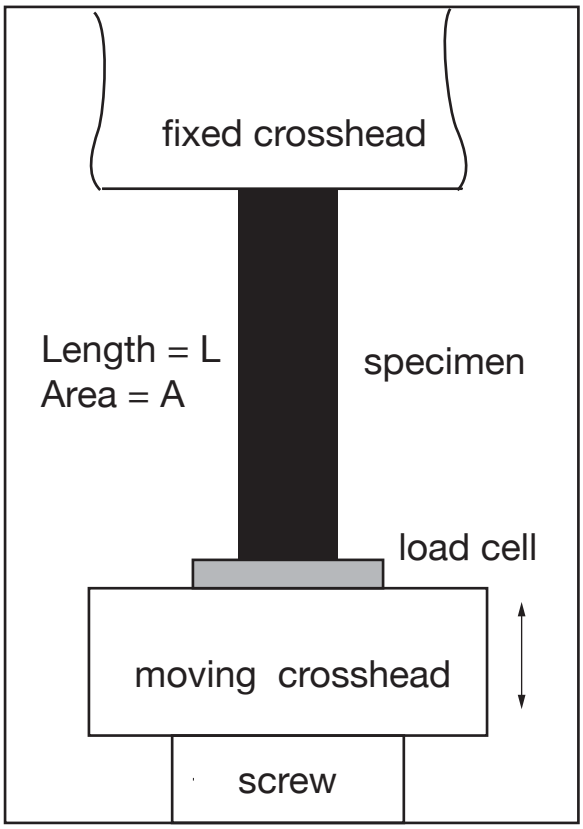
The Youngs modulus (E) is a good basis for normalizing the tensile strength of different materials to one another.

Since both E and the tensile strength must be related to the strength of bonds between atoms (and molecules), we seek to develop a simple model for relating them to each other.

Experiments suggest that the highest values of the tensile strength lie in the 5% to 25% of E. Can a simple model anticipate such fractions of the elastic modulus as an *upper bound* of the fracture strength.

The Youngs Modulus

The Instron Machine (shown on the right)



Uniaxial Stress

$\sigma = \frac{P}{A}$ units N m^{-2} or Pa

The experiment controls the displacement with the moving crosshead while the load cell measures the load.

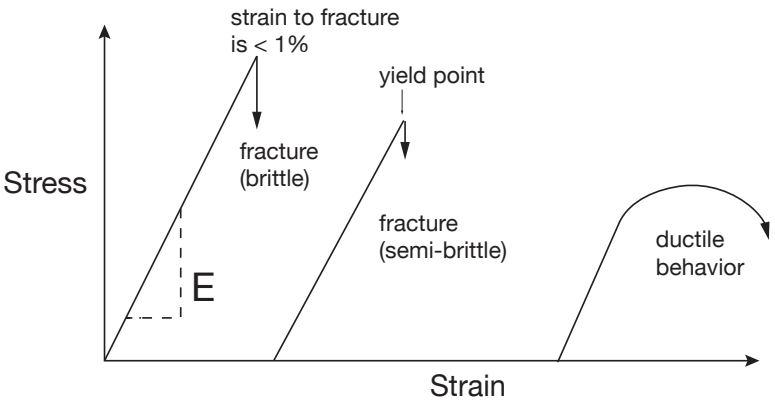
Uniaxial Strain

The P,u curve is converted into stress-strain curve

$\varepsilon = \frac{\Delta L}{L_o}$ (small strains - elastic deformation)

The Modulus

$E = \frac{d\sigma}{d\varepsilon} = \frac{\sigma}{\varepsilon}$ for linear stress-strain behavior.



Diamond has the highest modulus of all materials = 1000 GPa.

Graphite is a planar material which is very anisotropic. The graphene plane has high modulus, similar to diamond, while the out of plane modulus is far lower. Graphite fibers which are designed to have a high modulus are highly oriented assemblies of graphene sheets aligned in the fiber direction. Graphite reinforced polymer composites are constructed by such "graphite" fibers.

The modulus of several classes of materials is given in the map shown below.

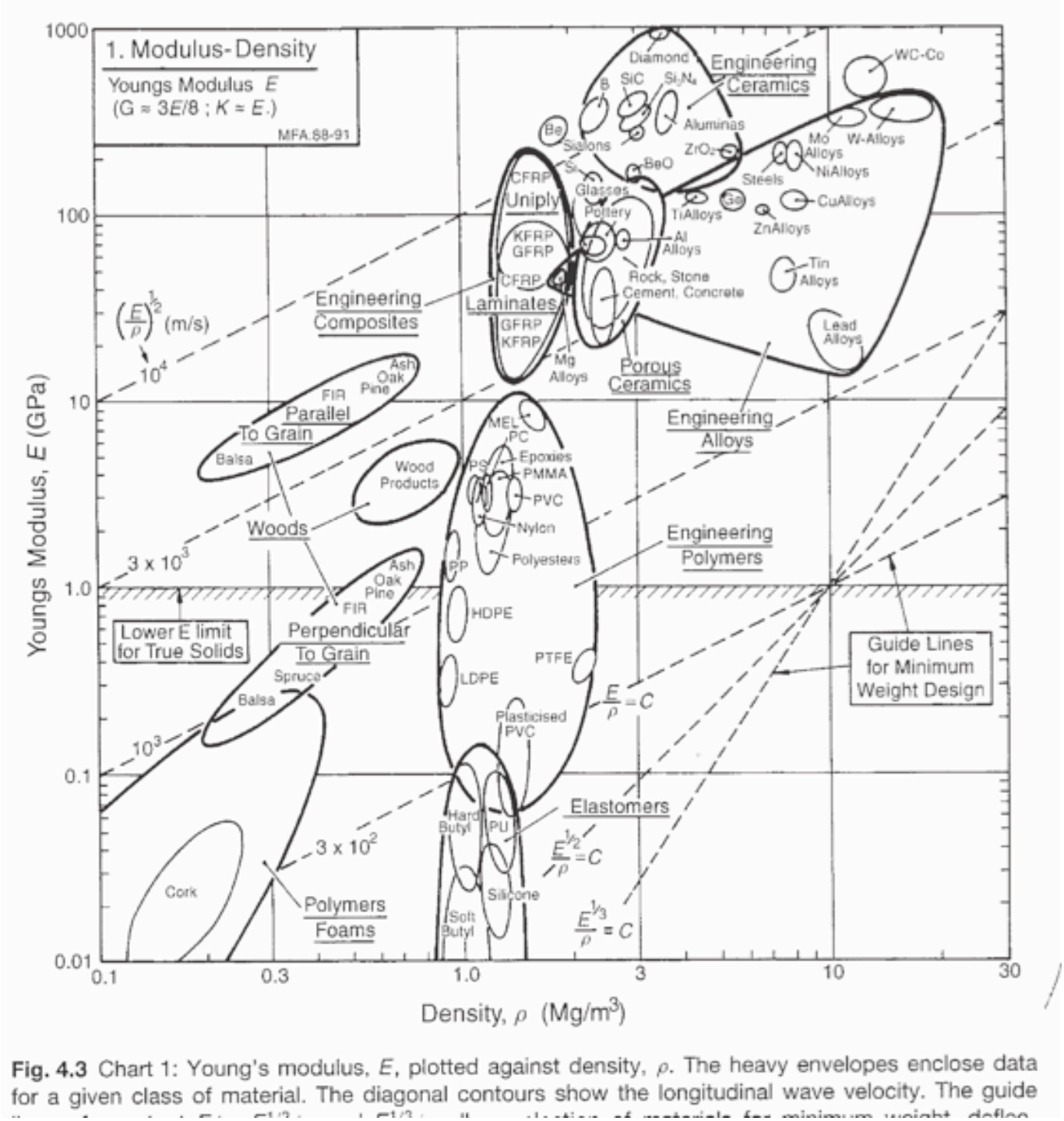


Fig. 4.3 Chart 1: Young's modulus, E, plotted against density, ρ. The heavy envelopes enclose data for a given class of material. The diagonal contours show the longitudinal wave velocity. The guide

Notes:

•Structural materials (metals and ceramics) lie at the top in the 100 - 1000 GPa range. Ceramics are usually above 500 GPa and metals are below 500 GPa.

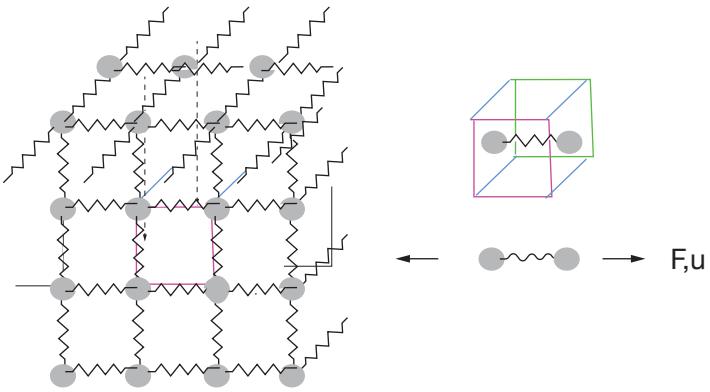
Bonds and Elastic Deformation

(i) Elastic deformation is reversible, that is, it recovers completely upon unloading.

(ii) Elastic deformation represents the stretching and recovery of ALL bonds in the solid. All bonds in the solid may be assumed to stretch in the same way.

(iii) The upper bound of the force when the bonds break, may be assumed to represent the "ideal" or the maximum fracture strength of the solid.

For simplicity we assume that the bonds are arranged in a cubic lattice.



Volume per atom = Ω

bond length = $\Omega^{1/3}$

cross section area per bond = $\Omega^{2/3}$

Stress: $\sigma = \dfrac{F}{\Omega^{2/3}}$

Strain: $\varepsilon = \dfrac{u}{\Omega^{1/3}}$

here u is the stretch displacement of the bond.

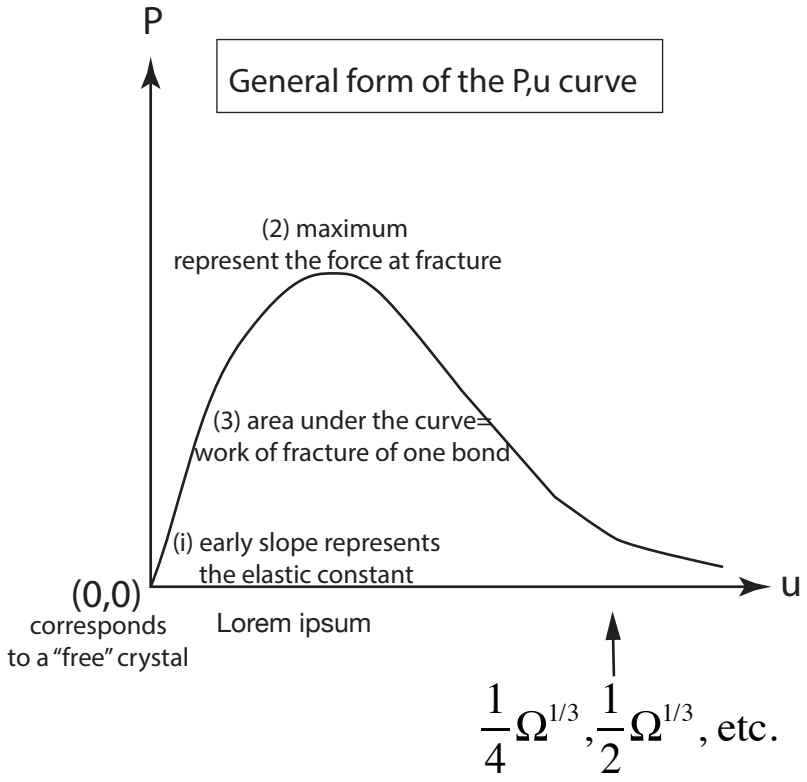
The Coordination Number

The cubic lattice assumption probably appears to be too severe. In a cube each atom has six nearest neighbors (NN). But often the number of NN can be greater: for example, it is eight in iron and up to 12 in simple close-packed structures. We manage this discrepancy by counting bonds which may be six, or eight or twelve. The number of NN are described as the coordination number, called Z. Therefore, the results we get for the simple cubic lattice can be extended to different degrees of packing of atoms by a factor $\dfrac{Z}{6}$ multiplied to the results obtained in the simple cubic case.

Thus, we may get a handle on the problem in a simple way.

Approximation for the Force Displacement Curve

We draw a force displacement curve for (F,u) from intuition. As shown in the spring model above the stretch on the bond between two neighboring atoms may be assumed to have the following form:



The shape of the curve shows that the force reaches a peak and the gradually falls away to zero when the atoms are pulled apart. Note that the bond does not break abruptly, but rather gives way gradually; this behavior is related to the electronic nature of bonding between atoms.

Atoms are constituted from a nucleus with a cloud of electrons around it. Bonds are created when atoms share electrons; the shared electrons spread out to spend time in each others orbits. Therefore when the atoms are pulled apart, the electrons slowly, and unwillingly part company. This way of disengaging gives rise to the gradual decline in the force that holds the atoms to each other.

The force-displacement curve shown above has three attributes:

- The slope at $u \to 0$, that is the slope at small displacements is the Elastic Modulus
- The maximum in the curve corresponds to the force required to "fracture" the bond
- The total area under the (P,u) curve is the work of fracture, or the energy of the bond measured mechanically

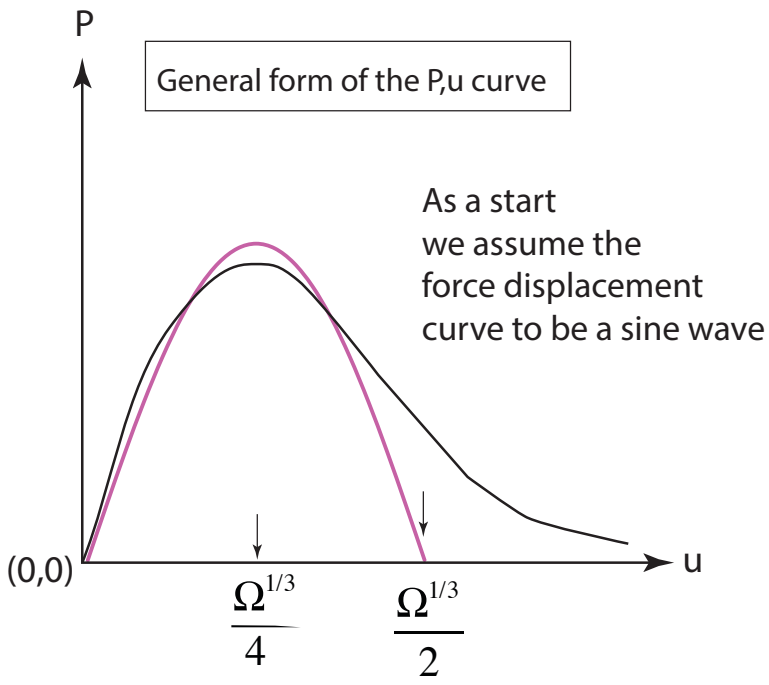
Adjustable Parameters in the Force-Displacement Curve

Clearly the parameters that describe the sketched force-displacement curve requires assumptions. For example,

- How far do the atoms have to be stretched until they are totally separated?
- Where is the maximum in the force that represent the ideal fracture strength?
- The u-axis in this curve should scale with the interatomic spacing, that is $\Omega^{1/3}$

The Sine-Wave Approximation

In order to enable a back-of-the-envelope analysis we assume a sinusoidal shape for the force displacement curve:



We are immediately required to make an assumption regarding the half wavelength of the Sine wave, that is the point where the force declines to zero. Again we resort to our intuition and assume that the force goes to zero when the bond had been stretched to twice its original length that is $\frac{\lambda}{2} = \frac{\Omega^{1/3}}{2}$, or that $\lambda = \Omega^{1/3}$ where λ is the wavelength of the sine wave shape.

With these assumption we may write an equation for the force displacement curve:

$$F = F_O \sin(\frac{2\pi u}{\Omega^{1/3}}) \qquad (1)$$

Here F_O is the maximum force that can be sustained by the bond. It is therefore also the highest possible fracture strength of the elastically deforming solid.

The Youngs modulus is now given by the early slope of the sine wave,

$$\left(\frac{dF}{du}\right)_{u\to 0} = \frac{2F_o\pi}{\Omega^{1/3}}\cos\left(\frac{2\pi u}{\Omega^{1/3}}\right)_{u\to 0} = \frac{2F_o\pi}{\Omega^{1/3}} \qquad (2)$$

Convert above into the Youngs modulus

$$E = \frac{d\sigma}{d\varepsilon} = \frac{d(F/\Omega^{2/3})}{d(u/\Omega^{1/3})} = \frac{dF}{du}\frac{1}{\Omega^{1/3}} = \frac{2F_o\pi}{\Omega^{2/3}} \tag{3}$$

$$\sigma_{ideal} = \frac{F_o}{\Omega^{2/3}} = \frac{E}{2\pi} \tag{4}$$

Note that $\frac{1}{2\pi} = 0.159$, that is the highest possible fracture strength will be about 15% of the elastic modulus.

The above result is a not an accident. It is a sensible approach that seeks to match theory to experiment. For example the wavelength can be adjusted to change the value of the upper bound (as a percent of the modulus).

The Work of Fracture

The total work done to separate the bond is equal to the area under the half sine wave:

$$\begin{aligned} &\text{Work per bond} = \int_0^{onehalfwavelength} F_o \sin\left(\frac{2\pi u}{\Omega^{1/3}}\right) \\ &U_{bond} = F_o \frac{\Omega^{1/3}}{2\pi}\left[-\cos\left(\frac{2\pi u}{\Omega^{1/3}}\right)\right]_0^{halfwavelength} \\ &= \frac{2F_0\Omega^{1/3}}{2\pi} = \frac{2\Omega^{1/3}}{2\pi}\frac{E\Omega^{2/3}}{2\pi} = \frac{E\Omega}{2\pi^2} \end{aligned} \tag{5}$$

Remember that the bond energy is shared between two atoms. Therefore the work done per atom per bond will be one half of value in Eq. (5).

Since each atom has Z nearest neighbors, the work that would be required to strip away the atom from the solid and make it free (like in a vapor state), which is also the enthalpy of formation, ΔH, will be given by

$$\begin{aligned} &\Delta H = \frac{U_{bond}Z}{2} N_A \text{energy of formation per mole} \\ &\Delta H = \frac{EV_{mole}}{4\pi^2} Z \end{aligned} \tag{6}$$

Note that the molar volume

$V_{mol} = \Omega N_A$ where N_A is the Avogadro's number. (7)

In Summary

$$\sigma_{ideal} = \frac{F_o}{\Omega^{2/3}} = \frac{E}{2\pi}, \qquad \Delta H = \frac{EV_{mole}}{4\pi^2} Z$$

We have related the ideal tensile strength to the elastic modulus, and the elastic modulus to the energy of formation (or the heat of evaporation).