

# ATOMISTIC BASIS OF ELASTICITY

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## Introduction

The *Introduction to Elastic Response* Module introduced two very important material properties, the ultimate tensile strength  $\sigma_f$  and the Young's modulus  $E$ . To the effective mechanical designer, these aren't just numerical parameters that are looked up in tables and plugged into equations. The very nature of the material is reflected in these properties, and designers who try to function without a sense of how the material really works are very apt to run into trouble. Whenever practical in these modules, we'll make an effort to put the material's mechanical properties in context with its processing and microstructure. This module will describe how for most engineering materials the modulus is controlled by the atomic bond energy function.

For most materials, the amount of stretching experienced by a tensile specimen under a small fixed load is controlled in a relatively simple way by the tightness of the chemical bonds at the atomic level, and this makes it possible to relate stiffness to the chemical architecture of the material. This is in contrast to more complicated mechanical properties such as fracture, which are controlled by a diverse combination of microscopic as well as molecular aspects of the material's internal structure and surface. Further, the stiffness of some materials — notably rubber — arises not from bond stiffness but from disordering or entropic factors. Some principal aspects of these atomistic views of elastic response are outlined in the sections to follow.

## Energetic effects

Chemical bonding between atoms can be viewed as arising from the electrostatic attraction between regions of positive and negative electronic charge. Materials can be classified based on the nature of these electrostatic forces, the three principal classes being

1. *Ionic materials*, such as NaCl, in which an electron is transferred from the less electronegative element (Na) to the more electronegative (Cl). The ions therefore differ by one electronic charge and are thus attracted to one another. Further, the two ions feel an attraction not only to each other but also to other oppositely charged ions in their vicinity; they also feel a repulsion from nearby ions of the same charge. Some ions may gain or lose more than one electron.
2. *Metallic materials*, such as iron and copper, in which one or more loosely bound outer electrons are released into a common pool which then acts to bind the positively charged atomic cores.

3. Covalent materials, such as diamond and polyethylene, in which atomic orbitals overlap to form a region of increased electronic charge to which both nuclei are attracted. This bond is directional, with each of the nuclear partners in the bond feeling an attraction to the negative region between them but not to any of the other atoms nearby.

In the case of ionic bonding, Coulomb's law of electrostatic attraction can be used to develop simple but effective relations for the bond stiffness. For ions of equal charge  $e$  the attractive force  $f_{attr}$  can be written:

$$f_{attr} = \frac{Ce^2}{r^2} \quad (1)$$

Here  $C$  is a conversion factor; For  $e$  in Coulombs,  $C = 8.988 \times 10^9 \text{ N}\cdot\text{m}^2/\text{Coul}^2$ . For singly ionized atoms,  $e = 1.602 \times 10^{-19} \text{ Coul}$  is the charge on an electron. The *energy* associated with the Coulombic attraction is obtained by integrating the force, which shows that the bond energy varies inversely with the separation distance:

$$U_{attr} = \int f_{attr} dr = \frac{-Ce^2}{r} \quad (2)$$

where the energy of atoms at infinite separation is taken as zero.

