ELECTRONIC BASIS OF THE STRENGTH OF MATERIALS

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Section II

Elements of solid mechanics

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Nature of elastic stiffness

The theory of elasticity is a structure of beauty and complexity. No one person sat down and wrote it out. From its first glimmerings in the mind of Galileo (ca. 1638) to the settlement of the question of the minimum number of coefficients required to specify a general elastic response took about 250 years. The latter work was done by Voigt (ca. 1888). Even then very little was known about the underlying factors that determine the coefficients; that is, the chemical properties that determine how resistant a material is to changes in its volume (the bulk modulus), and changes in its shape (the shear moduli). Even now the theory of shear moduli is only partially satisfactory.

Given the ongoing controversy regarding which comes first, practice or science, it is of interest to note that the early history of the theory of elasticity was motivated by the practical interests of those who made the important early advances. Leonardo da Vinci was interested in the design of arches. Galileo was concerned with naval architecture. Hooke wanted to make better clock springs. And Mariotte needed to build effective water piping to supply the palace at Versailles.

Complexity in the theory of elasticity is unavoidable because elastic behavior is intrinsically three-dimensional. Furthermore, most materials are not structurally isotropic; they have textures. Something as simple as a wooden post with a square cross-section looks different, in general, along each of the perpendiculars to its faces. These structural differences translate into different elastic stiffnesses in the three perpendicular directions. The situation is further complicated by the need to describe the shear responses in terms of a shear plane, plus a direction on the plane.

If forces are applied to the opposite ends of a slender bar, it will elongate or contract in proportion to the size of the forces (Hooke's Law). The coefficient of response is Young's modulus. However, the bar might also be twisted around its length, or it might be bent around an axis perpendicular to its length. The twisting mode of deformation requires another response coefficient, the shear modulus. If the slenderness of the bar is reduced to the limit of a line, both of its elastic moduli become meaningless. They cannot exist in the absence of finite atoms, and the bonds between the atoms which are formed by electrons that behave according to quantum mechanics.

Consider a square mesh of wires soldered together at the intersections of the wires (a wire screen). Suppose a square piece is cut from the mesh with the edges of the square parallel to the wires. If forces are applied parallel to the edges of the square, the response will be stiff, whereas if forces are applied parallel to one of the diagonals of the square, the response will be relatively soft. Thus two distinctly different response coefficients are needed to describe the square's mechanical behavior.

Next imagine a three-dimensional framework of wires in a cubic array soldered together at the nodes of the wires (on a larger scale this would be like the framework of a steel building with all of the girders of the same length). This will have three different response coefficients in general: one for forces applied parallel to the wires, another for forces applied parallel to the diagonals of the faces of the cubes, and the third for forces applied along the diagonals of the cubes (lines connecting the opposite far corners). The three coefficients can be reduced to two by adjusting the design of the nodes; then the structure is said to be elastically isotropic.

More response coefficients will be required if the symmetry of the structure is less than that of a cube. For example, if the framework consists of rectangular parallelepipeds, the number of coefficients increases to nine (orthorhombic symmetry). Then if the number of different lengths is reduced from three to two (tetragonal symmetry), the number of coefficients drops from nine to six; and if the number of different lengths is further reduced to one, only three coefficients are needed (cubic symmetry) as already indicated.

Clearly, a standardized framework is necessary within which the elastic coefficients can be defined. This is provided by tensor calculus which, as the name suggests, was devised for this purpose. It is necessarily more complex than vector calculus because the elastic state of a solid requires both tensions (or compressions) and shears to describe it.

The first step is to define what is meant by *stress* and by *strain*. This will include a definition of the notation that is used to distinguish the various possible components of the stress and strain tensors. Then the response coefficients that connect them can be defined.

One of the purposes of this book is to show how the response coefficients (elastic constants) are determined by the chemical and physical constitutions of various solids. This involves the interior geometry of the solid, and its corresponding electronic structure.

Temperature and time both have small and large effects on elastic stiffness depending on the material. At very low temperatures elastic stiffness becomes independent of temperature, but at higher temperatures (near the Debye temperature and above) various *anelastic* effects occur. Then a given material has two stiffnesses: one for fast loading when there is too little time for anelastic relaxation (called the unrelaxed modulus), and the other for slow loading which allows relaxation to occur (called the relaxed modulus). The difference between these two stiffnesses is small for solids in which the atoms are densely packed. A much larger effect is found in less dense materials such as elastomers (rubber-like materials). In these, the molecules tend to curl up into coils which have high entropy because they can be formed in many different ways. When applied tractions stretch them, there are fewer ways for them to coil so their entropies decrease. This increases their free energies, so they resist stretching, but relatively weakly. They are sometimes said to have “entropic elasticity”, as contrasted with the more usual “enthalpic elasticity”.

The elastic response coefficients are the most fundamental of all of the properties of solids, and the most important sub-set of them is the shear coefficients. If these were not sufficiently large, all matter would be liquid-like. There would be no aeronautical, civil, or mechanical engineering. Furthermore, modern micro-electronics, as well as opto-electronics would not be possible. The elastic stiffnesses set limits on how strong materials can be, how slowly geological processes occur, and how natural structures respond to wind and rain. This is why the scientific study that began with Galileo continues today.

Imagine a world in which everything has the same elastic stiffness. If all the bulk stiffnesses (the resistance to volume changes) were the same, nails could not be driven into wood, and plows could not turn earth. Or, suppose that the stiffness of aluminum were one-fifth as large as it actually is. Then the wing tips of large aircraft would drag on the ground because the elastic deflections would be so large. It is for reasons like these that the elastic properties of solids have great engineering significance, and why the theory of elasticity played such an important role in the histories of both engineering and physics.

The architecture of the theory of elasticity is now considered to be applied mathematics, but once was in the mainstream of the development of calculus and differential equations, as well as physics. For a long time (centuries), the elastic properties were coefficients to be measured and tabulated. Their relationship to the properties of atomic particles, and to one another, awaited the development of quantum mechanics. Although there remain some aspects of the theory that are not entirely satisfactory, the progress that has been made toward a general theory is impressive.

All forms of matter (gases, liquids, solids, plasmas, etc.) resist changes of volume, and the amount of this resistance is measured by means of the bulk modulus. Its inverse is the compressibility. Solids are defined by their shear stiffness moduli. These have inverses called shear compliances. Since the shear response is difficult to separate from the volumetric response, the overall description of elastic behavior is complicated.

The primary factor determining elastic stiffness is chemical constitution because it determines the internal bonding. Broadly, there are four kinds of bonding: covalent, ionic, metallic, and molecular. Each has its idiosyncrasies. The stiffest bonds are of covalent character, while the least stiff are molecular.

In addition to their shear stiffnesses, solids have another special feature. They can be either perfect, nearly perfect, or imperfect, in terms of their structural geometry. An ideal, or perfect, solid has a specific crystal structure, and each site of the crystal structure is occupied by a specific atomic species. However, virtually all solids contain defects, including thermal vibrations, vacancies, interstitials, impurity atoms, dislocations, stacking faults, domain boundaries, and grain boundaries. These affect the elastic stiffness, particularly the shear stiffness.

The time dependence of elasticity, or *anelastic* response, results from a variety of effects. Some of these are the thermo-elastic effect, the hopping of carbon atoms in iron (Snoek effect), and the stress-induced ordering of atomic pairs in some alloys. The anelasticity of elastomers (rubber) is a much larger effect.

Changes of shape (strains) can be induced by fields other than stresses. Electric fields cause electrostriction, or piezoelectric strains; and magnetic fields cause magnetostriction.

An aim here is to describe the connections of the various response coefficients to chemical constitution. This is unlike many books on strength which describe the field variables, leaving the elastic stiffnesses as coefficients to be measured and tabulated.