ELECTRONIC BASIS OF THE STRENGTH OF MATERIALS

This book is the first to relate the complete set of strength characteristics to the electronic structures of the constituent atoms. These relationships require knowledge of both the chemistry and physics of materials. Also, the book uses both classical and quantum mechanics since both are needed to describe the properties of atoms. The book begins with short reviews of the two mechanics. Following these reviews, the three major branches of the strength of materials are given their own sections. They are: the elastic stiffnesses; the plastic responses; and the nature of fracture.

Elastic deformation can be reduced to two pure types: volume changes, and shape changes (shears). The moduli (stiffnesses) associated with each of these can be quantitatively obtained by means of the Heisenberg Principle and the theory of polarizability. The analytic theories are simple enough to indicate the physical origins of these properties. The most important atomic properties are the valence electron densities, and the electronic polarizabilities. These lead to electron exchange forces, and photon exchange forces, respectively. Atomic, molecular, and plasmonic polarizabilities play important roles. The anomalously large shear stiffness of diamond is explained in terms of the distribution of electrons along the covalent bonds, resulting from electron correlation.

For plastic deformation, the critical role of dislocation mobility is discussed. In nearly perfect metal crystals (and ionic salts) there is no quasi-static resistance to dislocation motion (only electron and phonon viscosity). Resistance in imperfect crystals is caused by extrinsic factors. In nearly perfect covalent crystals (semiconductors), dislocation mobility is intrinsically limited by the localized chemical bonds. Using diamond as the prototype, a quantitative theory of intrinsic mobility is presented.

Fracture is discussed in terms of intrinsic surface energies and their effects on the fracture surface energies of real materials. Two simple approaches are discussed. One is based on the Heisenberg Principle, the other on the plasmon theory of Schmit and Lucas. The latter may be important for understanding ductility.

This book presents a comprehensive view of the relationships between the electronic structures of solids and the microscopic and macroscopic mechanical properties of solid materials. It will be of great value to academic and industrial research workers in the sciences of metallurgy, ceramics, micro-electronics, and polymers. It will serve well as a supplementary text for the teaching of solid mechanics.

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Preface

In the middle of the twentieth century it was recognized that the theory of the mechanics of continua (particularly solid mechanics) is not adequate to account for the strength properties of materials. It was clear that structural considerations at the microscopic and nanoscopic levels of aggregation are not only important but are essential to an understanding of the strengths of materials. It also came to be realized, as a result of the fact that plastic shear deformation is usually heterogeneous, that a space can be continuous but not simply connected, that is, dislocated. Also, in crystals, such dislocations are quantized, having constant displacements equal to the magnitudes of translation vectors of the crystal structure.

Although structural geometry plays an essential role in determining mechanical behavior, it leaves a number of questions unanswered. The answers to these questions can only be found by considering the electronic structure that underlies the geometric factors. Since the behavior of electrons is not described by classical mechanics, this necessitates the use of quantum mechanics to obtain answers to the various unanswered questions. For example, why is the shear stiffness of diamond greater than its volumetric stiffness? Why do the most simple metals, the alkalis, have body-centered cubic crystal structures which are not atomically close packed? Why is pure silicon brittle, while pure nickel is quite ductile? They both have the same crystal structure, so why is pure TiC hard, while pure NaCl is soft? Why do intermetallic compounds often change their color when they are plastically deformed? What determines the temperature dependences of yield stresses? Why are grain boundaries weak? What activates plastic flow and crack growth at low temperatures where there are no thermal fluctuations? Only the subatomic behavior of electrons can account for these phenomena. This is the theme of this book.

I recall seeing a review of a book (*Electronic Structure and the Properties of Solids*) by Walter Harrison that called it "idiosyncratic". It is that, but it is also comprehensive and instructive as only a lifetime of scholarship could make it. This book is also idiosyncratic. That is, it is one person's view of a vast and complex subject. Whether it is instructive is a verdict to be brought by readers.

This book differs from most books dealing with electronic structure which introduce the formalities of quantum mechanics, and then circumvent them with approximations and numerical computations. Here, it is assumed that solids are so complex that it is better to make the approximations first, and then try to show that they are consistent with the basic

rules of quantum mechanics, and that they yield properties consistent with the measured values. In this regard much use is made of Heisenberg's Theorem in its exact form, so there is nothing uncertain about it. It is an approximate solution of Schrödinger's equation.

Perhaps the most controversial topic in the book is that of dislocation mobility. Together with W.G. Johnston, the author made the first direct measurements of dislocation mobility, and therefore has some knowledge of its intricacies. The latter have not been described consistently in much of the extant literature. A purpose of this book is to correct this.

Sometimes explicitly, and often implicitly, the electronic properties on which the strength properties depend are the valence charge density, and the electronic polarizability. The reader should have a better appreciation of this after reading this book. Since these are also the electronic properties that primarily determine the optical and the chemical properties, this demonstrates the unity that exists among the various properties.