

Mechanical Properties of Metals

**Atomistic and Fractal
Continuum Approaches**

金属的力学性能

**C W Lung
N H March**

World Scientific

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Preface

This book aims to bring together continuum elasticity theory, electronic structure and the concept of fractals as applied to roughness and toughness of metals.

Of course, a major contribution to fracture was made by Griffith, in which, though incomplete for reasons that are now largely understood, he derived an expression for the limiting strength of a material. This involved intimately the surface energy, which subsequently, at least in a simple metal like Al with s and p electrons, has been related to the energy of formation of a vacancy. However, a tremendous step forward came with the concept of a dislocation.

It was shown that if a limited area of one plane slips by one atomic distance over the neighbouring plane, the boundary of this area is a closed loop of dislocation. Once this loop is formed, glide can propagate across the plane by the spreading of the area, which is a motion of the dislocation line across its glide plane. General interest in dislocation theory was aroused by its success in providing atomistic theories for plastic deformation and crystal growth. Progress has been made in this field for more than one decade on the treatment of elastic anisotropy and dislocation mobility. For more than two decades, interests have concentrated on deepening our understanding of the structure and role of the dislocation core the behaviour of a pile-up of dislocations (simulating a crack). Interatomic forces (electronic structure) play a decisive role in the structure of the dislocation core and even in fracture. In particular, the temperature dependence of fracture toughness of materials has a close relationship to the interatomic forces. Molecular dynamics has been applied to understand the dislocation motion and the emission of dislocations at the crack tip under loading. Dynamics of crack propagation has become an area of considerable current interest for theoretical physicists and material scientists.

As to electronic structure, electron density theory based on a one-body potential $V(\mathbf{r})$ including electron-electron exchange and correlation interactions has transformed what can be done on electronic structure of both perfect and

defective crystals. Nevertheless, it is still important to subsume ideas involved there into interatomic force fields, which can then be used to study extended defects such as surfaces, grain boundaries, dislocations and cracks. There is still, however, much to do in understanding, in metals, the role of collective effects (including plasmons) in determining mechanical properties and tribology of conducting materials. If our book proves to make a contribution to furthering the progress in relating and enriching ideas from continuum theory, from electronic structure, and from concepts of fractal structure, then that will be more than ample justification for the effort involved in the present project.

We are conscious that in some areas embraced in our book, there is rapid movement at the time of writing. If authors in electron theory or in very practical aspects of materials science and engineering see where we ought to do better, we shall count it a privilege if they write to us with positive suggestions for improvement.

Over a decade or more, diverse scientists have recognized that many of the structures common in their experiments have a special kind of geometrical complexity. Mandelbrot in his pioneering work introduced the concept of fractals and used the idea of a fractal dimension which often is not an integer to characterize the complex structure quantitatively. Fractals may be considered as systems which obey the law of self-similarity, or are self-affine.

Since Mandelbrot *et al.* (1984) showed that fractured surfaces are fractals in nature and that the fractal dimensions of the surfaces correlate well with the toughness of the material, many authors have found that the fractal dimension depends on the fracture properties of materials, but the values of it seem in a narrow range for measurements with a resolution down to the micron scale. This has led to much discussion on the universality and specificity of the fractal dimension of fractured surfaces. However, the roughness index (or local fractal dimension) is found to display wide differences depending on materials on a small length scale by means of scanning electron microscopy (SEM). Another problem is that the negative correlation of the fractal dimension of fractured surfaces with toughness of ductile materials is quite difficult to understand. These basic problems remain open at the time of writing and much remains to be done.

We could not end this Preface without acknowledging our indebtedness to other workers. C. W. Lung wishes to thank Professor P. L. Zhang for leading him into active research in materials physics, Professors T. S. Ge(Kê) and K. X. Guo for their advice, collaboration and much practical support, and Professors H. Wu, X. Li, J. Z. Gao and C. X. Shi for their continuous encouragement.

N. H. March is greatly indebted to Professor J. A. Alonso for many invaluable discussions on electrons in metals and alloys. Professor A. B. Lidiard played a prime role in interesting N. H. March in the problems of materials science and he is thanked here for the great influence he has thereby had on the present project. Dr. P. Schmidt has given N. H. March much encouragement and stimulation in his work in this field and support from the Office of Naval Research (ONR) is gratefully acknowledged. We are especially grateful to Professor V. Vitek for his permission to draw heavily on his lectures at the International Centre for Theoretical Physics (ICTP) in Trieste and from his contributions to a NATO Advanced Study Institute. The authors first met at ICTP Trieste, and much of their collaboration has resulted from frequent summer visits there. They thank Professors A. Salam and M. A. Virasoro for much hospitality. We thank also the many researchers who have sent us papers and have thereby helped us in preparing the book. Last, but not least, Ms G. Su has skilfully typed most of the manuscript and we are very grateful to her.

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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.