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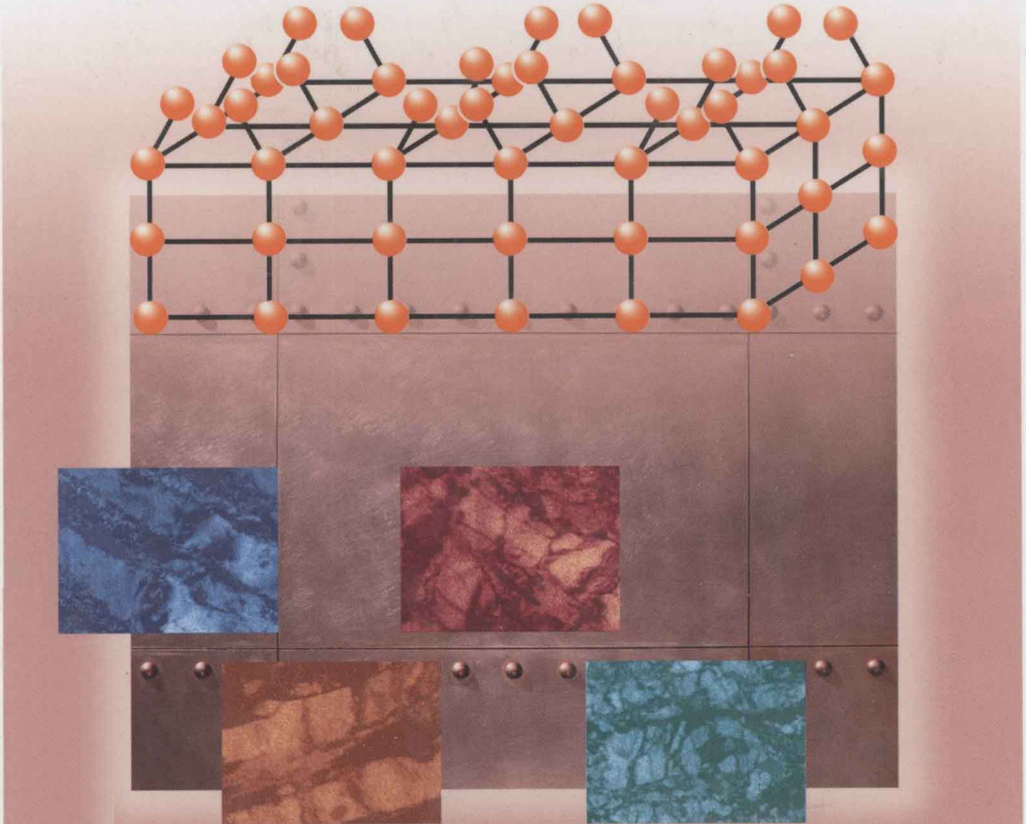
Theory, Nanostructuring and Fatigue Strength



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Introduction

The properties of surface layers of solids are of fundamental importance in solid state theory.

A considerable body of evidence shows that atoms in surface layers exist under different conditions from the state of bulk atoms. It is the breaking of interatomic bonds near the surface that determines the special conditions on the surface. The arrangement of atoms at the surface is the key factor which affects the physical, mechanical and chemical properties of metallic materials and other solids, especially semiconductors and chemical compounds. The broken atom bonds cause distinct changes in the distribution of electrons.

On the other hand, surface layers play an important role in the behavior of solids in practical applications. Numerous technological processes influence the special properties of surface layers. Any strengthening or treatment of solids begins with the surface. An optimization of the surface microstructure allows one to produce materials with a nanocrystalline surface layer.

In turn, cracks, wear and rupture arise from the surface under normal operating conditions. Adsorption and chemical reactions also begin on the surface.

Fatigue rupture and the high-temperature creep originate in surface layers. The structure of the surface is responsible for fatigue strength, corrosion resistance, and wearing capacity. Surface layers contain defects of different dimensions, e.g. vacancies, dislocations, distortions, steps, adsorbed atoms.

Over recent decades, physics has made significant progress in the study of surfaces of metals, alloys, and semiconductors on a microscopic scale.

It is helpful to make the study of surfaces as simple as possible by eliminating extraneous factors. From the physical point of view it is necessary to investigate an ideal clean surface.

In order to keep the surface fairly clean specimens need to be in an ultra-high vacuum. One should keep the residual gas pressure lower than 10^{-8} Pa (7.5×10^{-11} Torr) for a long time. Vacuum physics and technology gave a strong impetus to surface science. The preparation of well-defined, clean surfaces, which are usually investigated, became possible only after the development of the ultra-high vacuum technique.

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However, the majority of industrial processes occur in the atmosphere. Real parts and components operate under usual atmospheric conditions. Most scientists and engineers do not find an ideal and absolutely pure solids surface. Deformation distortions, chemical impurities, and absorption layers are typical for solid surfaces, in reality. These facts substantiate the investigation of surfaces in non-ideal conditions.

The main goal of our book is the study of strained metallic surfaces under ordinary conditions.

A strained state of the metallic surface is the outcome of prior treatment and manufacture.

Residual stresses are produced by plastic deformation, thermal contractions or can be induced by a production process. The residual mechanical stresses are known to balance in the macroscopic and microscopic areas of materials. The plastic strain of the surface is well-known in the industry as a way to improve the fatigue and strength properties of metallic parts. Shot peening, deep rolling, hammering, treatment by metallic balls in an ultrasonic field, and laser shock peening are the new technological methods used to increase the strength of crucial parts. All these processes somehow or other induce the near-surface nanostructures. The generation of nanostructured surface layers is expected to improve the properties of materials. Structural changes in the near-surface regions of metals and alloys are of great interest and have not yet been sufficiently investigated.

The electronic work function is of special and increasing interest to material scientists and engineers because of its sensitivity to the physical state of the surface. Metals are known to consist of two subsystems. These are the relatively slow crystal lattice of ions and the gas of the fast free electrons. External and residual stresses result in considerable changes in the ionic crystal lattice.

The properties of electron emission indicate close interaction between ionic and electronic subsystems. It is essential, however, to emphasize that a relationship between the emission properties and elastic and plastic strain is not yet sufficiently understood. Here we would like to make up for this deficiency of data.

The vast development of surface science has been covered in many excellent books on the technique of surface investigation, surface structure, surface processes, and the theoretical modeling of the surface. Previous investigations and books have deepened our knowledge on the problem and stimulated much experimental work. However, there is a gap in the existing literature. It is preferable to study pure metals in theoretical investigations. The physical fundamentals of surface deformation, especially of industrial nickel-based superalloys and titanium-based alloys, are not clearly understood.

We believe there is a need for a book to act as a bridge between a theory and its practical applications. This book is an attempt to bridge the gap between surface physics and physics of solids and technology. Our goal is to consider physical theories as well as the applied aspects of the strained surface problem.

The book treats data from systematic experimental measurements of important characteristics which are related to physical fundamentals of peculiarities of strained metallic surfaces. The book is designed to cover data accumulated during recent decades when studying the properties of these surfaces.

The lower layers of the solid surface are involved in deformation processes, as well as the top ones. In this book the metallic surface is regarded as the top of tens of atomic layers.

The book consists of eleven chapters.

A succinct description of the features of the metallic surface is presented in the first chapter. We recall the concepts of surface energy and surface stress. The defects at the surface are discussed. We describe the crystal structure of the surface and the distribution of free electrons near the surface. We would also like to remind the reader of the quantum phenomena related to the surface.

The second chapter is devoted to some techniques for experimental studies of the strained metallic surfaces. Diffraction methods are considered. We describe the technique of precise X-ray measurements of residual macroscopic stresses. A new installation and the method of measurement of the electronic work function are presented. Attention is given also to mechanical methods of studying of the surface layers. The materials under investigation are described.

The emission properties of the strained metallic surface are the subject of the third chapter. A scanning Kelvin probe method is used to investigate the strained and stressed surface of metals and alloys. Data on the response of the electronic work function to the elastic and plastic deformation of metals are presented and discussed. The physical mechanism of processes is deduced from the results obtained and the phenomena responsible for the variation in the work function are discussed.

The fourth chapter deals with an examination of various models of the electronic work function for the strained surface. Some theoretical models are proposed. Equations are derived for the calculation of the electronic work function of the imperfect surface and methods of calculation of the work function of the elastic strained metal surface, are developed. A theoretical basis for this consideration is a self-consistent scheme of the work function calculation which took into account essential corrections to the jellium model as well as the formation of nanometric surface defects.

In the fifth chapter we consider the contact interaction of metallic surfaces which is inherent in processes of wear and tear, mechanical treatment and strengthening. The technique of local indentation which is one of the effective methods of measurement of properties of the materials considered. The work function procedure is found to be sensitive to processes of friction and wear.

Data on the fatigue prediction for metals and alloys are presented in the sixth chapter. The basic mechanism of fatigue fracture is the origination of a crack on the surface and a slow propagating of the crack. Fatigue of materials is known to be a dangerous phenomenon. We discover that the nondestructive method of work function measurement may be used to predict the initiation of fatigue cracks.

The seventh chapter contains a computer stimulation of the evolution of structure parameters during fatigue. We work out a physical model that describes processes leading to fatigue. Our approach is to derive a system of ordinary differential equations and to solve the system numerically.

The eighth chapter deals with data on surface residual stresses and fatigue life of gas-turbine components. The need to use high stresses in aircraft causes initiation of fatigue cracks. The induced favorable residual stresses are used in industry to increase the fatigue strength. The authors present their results of the study of gas-turbine blades and discs. In this chapter we consider the distribution of induced macroscopic residual stresses for real engine parts and the effect of surface treatments on the fatigue strength. Microscopic stresses and subgrain sizes are also measured.

The ninth chapter contains a considerable body of evidence on nanostructuring and strengthening of metallic surfaces. Various mechanical treatments of the surface and induced nanometric structures are considered. Favorable structural factors which have a significant influence on fatigue life and lead to additional increase in fatigue strength are also discussed. We describe the distribution of residual stresses with the depth, their evolution during fatigue tests, and the stability of the microstructure during cycling. Semi-empirical models of fatigue behavior are presented.

In the tenth chapter we derive a quantitative physical mechanism for fatigue. The fatigue phenomenon is considered on the atomic scale. We discover that fatigue damage is, at first, reversible. The initiation and propagation of fatigue cracks are under study. We place an emphasis on the role of the crack growth of vacancy flow and of the stress gradient near the crack tip. Periods of the fatigue damage are considered from the physical point of view. A focus is placed on the dependence of the crack growth rate on the cycling time and the stress amplitude. We derive equations for the assessment of embryo crack length, and number of cycles until specimen fracture.

In the eleventh chapter we consider some new methods of fatigue life prolongation. Topics that are discussed concern the intermediate thermal treatment, the processing of alloys by electric impulses, and a combined strengthening of compressor blades. This consists of the restoring of components, the severe plastic strain of the surface, and the armoring of blades by a coating. We discuss also structure elements of fatigue performance.

A detailed review of all aspects of the problem under consideration for a pure ideal surface goes beyond the scope of this book. Therefore, the known principles and established facts are mentioned only briefly. The reader can find reviews concerning the physics of ideal surfaces in different books and articles, for example [1-8].

This book is intended for students and postgraduate students in the area of solid state physics, surface physics, materials engineering, and physical chemistry. At the graduate and postgraduate level there is reason to believe that the book will meet the needs of those concerned with the properties, investigation and application of modern industrial alloys.

We hope that the book will also be useful for material scientists, engineers, researchers and practitioners from the industry sectors who are interested in problems of material properties, surface strengthening, nanostructuring, fatigue strength, and physicochemical activity.

1
Peculiarities of the Metallic Surface

1.1
Surface Energy and Surface Stress

The first law of thermodynamics states that

$$dQ = dU + dW \tag{1.1}$$

where dQ is the increment in the heat energy of the system, dU is the increment in the internal energy and dW is a work that the system has performed. Only dU is the total differential and it is independent of the method of system transition from one state to another.[1] dQ and dW are simply infinitesimal quantities. In fact, (1.1) is the law of the energy conservation for an isolated system.

Substituting $dQ = T\,dS$ and $dW = p\,dV$ in (1.1) one arrives at

$$dU = T\,dS - p\,dV \tag{1.2}$$

where S is the entropy, T is the temperature, p is the pressure, V is volume of the system.

The internal energy of the system depends also on the number N of particles, that is, atoms or molecules. Thus, one should add the corresponding term:

$$dU = T\,dS - p\,dV + \mu\,dN \tag{1.3}$$

where μ is the chemical potential. The chemical potential is defined as a change in the internal energy when the number of particles varies at constant entropy and volume:

$$\mu = \left(\frac{\partial U}{\partial N}\right)_{S,V} \tag{1.4}$$

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[1] If the internal energy is a function of the pressure and the temperature, $U = U(p, T)$, then the infinitesimal increment in the internal energy is given by $dU = \left(\frac{\partial U}{\partial p}\right)_T dp + \left(\frac{\partial U}{\partial T}\right)_p dT$.

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The internal energy U increases (or, on the contrary, decreases) if

- the system receives (returns) the heat or
- mechanical work is done under the system (the system does mechanical work) or
- the number of particles in the system increases (decreases).

Turning to the free energy. The Helmholtz free energy F is known to be equal to

$$F = U - TS \tag{1.5}$$

Differentiating (1.5) and combining with (1.3) we obtain

$$dF = -S\,dT - p\,dV + \mu\,dN \tag{1.6}$$

At constant temperature and volume the increment in the free energy varies linearly with increase in the particle number,

$$dF = \mu\,dN \tag{1.7}$$

with the proportionality factor $\mu = \mu(T, V)$.

The Gibbs thermodynamic potential $G = F + pV$ is expressed as

$$dG = -S\,dT + V\,dp + \mu\,dN \tag{1.8}$$

The difference between the Helmholtz free energy and the Gibbs thermodynamic potential is insignificant under atmospheric pressure for a bulk solid.

Molecules of the surface layer in a homogeneous liquid are known to be attracted by other molecules within the liquid. Unlike in the body of the liquid the attraction of surface molecules is not compensated. Liquids turn out to be covered by an elastic stretched film and so the concept of surface tension is used for them.

The thermodynamic approach can also be applied to the surface of solids. J. W. Gibbs was the first to note that the surface contributes to the free energy. He also considered the cleavage process of a bulk body.

In order to create a free surface one must break the bonds between neighboring atoms. This implies that the creation of an additional piece of surface costs the system extra energy. The surface energy is equal to the work necessary in order to form the unit area of surface by a process of division of the solid into parts. This process is assumed to be thermodynamically reversible.

The reversible work dW required for an external force to create an infinitesimal area dA of the surface is directly proportional to this area

$$-dW = \gamma\,dA \tag{1.9}$$

where γ is a proportionality factor. It is dependent on temperature, volume, and the particle number.