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Physical Foundations of Materials Science

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With 472 Figures

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To Norma, Björn, Jan, and David

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Preface

This book is a translation of a German textbook on Materials Science. It originates from a set of handouts at the RWTH Aachen university for students of materials engineering and of metal physics and was developed over the years to a compact manuscript. From the core of a physical metallurgy text it was extended to a broader coverage of materials in the frame of established scientific concepts.

The text aims at providing the physical fundamentals to understand materials behavior and at preparing the reader for more advanced litarature on the subject. On the other hand the book is designed not to follow the common scheme of traditional introductory Materials Science texts which primarily introduce into the phenomenology of materials on an elementary level. Rather this book tries to bridge the scope from atomistic mechanisms to engineering properties of materials not staying away from mathematics where necessary. The manuscript does not pretend to give a comprehensive coverage of materials science, and as a textbook it has to find a compromise between comprehensive and in depth treatment of the subject. Such compromise is a matter of personal preference and taste. This is particularly true for the chapter on "physical properties" which is designed for materials engineering students who usually are less familiar with the basics of solid state physics.

The text builds on the classical German text of Masing "Einführung in die Metallkunde" (introduction to physical metallurgy) which represents the approach of the Göttingen school of physical metallurgy in the line of Tammann, Masing, Haasen, and Lücke. It is typical for this approach to develop a deeper understanding of the subject and to reduce complex phenomena to their essential physical mechanisms for refined analysis and prediction. Since understanding is essentially based on visualization the text provides an abundance of figures to guide the reader through the seemingly confusing but fascinating world of materials.

Contents

Introduction

The development of new materials is considered a key technology on an international level. The capability of production, fabrication, and application of high performance materials is a prerequisite for novel, and internationally competitive products and processes and a crucial element for more efficient use of resources and for environmental protection.

The development of novel materials and processes requires a deep knowledge of the physical foundations of materials as a tool for systematic tayloring of materials properties. These physical foundations are the roots of material science, and they are the key elements of this text book. The term material science is relatively young and not very precisely defined. Sometimes it is understood as an extension of physical metallurgy to non-metallic materials. Natural scientists frequently associate material science only with novel or even exotic functional materials.

In the following we will define materials science as our knowledge of the relation between microscopic structure and macroscopic properties of engineering materials. It combines the broad spectrum of commercially utilized solids ranging from metals to ceramics, glasses, and plastics to composites and electronic materials.

The most important group of engineering materials, both with respect to production volume and variety of applications as well as tradition and systematic development, are metals. Their excellent combination of formability and strength have made them prime materials for structural applications and their excellent electrical and thermal conductivity has rendered them indispensible for electrical engineering. Metals have determined the history and development of materials over several thousand years, even coined the names of historical periods like the bronze age which dates back to 3000BC. The need for low cost mass products and components for extreme service conditions in our industrial age have made high performance ceramics, plastics, and eventually composites highly compatitive materials.

The materials science of ceramics, plastics, and electronic materials is relatively young compared to metallurgy. The physical foundations and theoretical concepts of metals, ceramics, semi-conductors, and plastics, however, share a large common frame, which is essentially derived from the foundations of physical metallurgy. In this respect, metallurgy is the mother of materials science as evident from the extensive research in this class of material over many centuries. Despite its very long tradition, metallurgy is not a classical scientific discipline itself. Up to medieval ages knowledge of the extraction and fabrication of metals had been considered a national secret asset and had been only traded orally from generation to generation. Only in the middleages a German metallurgist of name Bauer (engl. farmer, in latin "Agricola") wrote down the recipes of metal fabrication in his famous book "De Re Metallica" [0.1]. The book reads like a mystic instruction to metal fabrication, there is mention of bull blood and clear nights of full moon, harmful creatures like cobolds and nickels (therefore the terms cobalt and nickel) all of which had practical relevance, e.g. for making a steel harder, and which we explain nowadays on a scientific basis. As a matter of fact metallurgy was a discipline of alchemie in medieval times and comprised a colorful mixture of empirical recipies and superstition.

With increasing scientific character of more recent centuries metallurgy became a displine of chemistry, where it remained even up to now at many universities. The rapid development of the understanding of materials properties, in particular due to the discovery of X-rays and their application to crystallography, revealed that the properties of metals were not determined by the gross chemical composition, in contrast to common belief at that time. This made metallurgy to become a discipline of physical chemistry. The development of the atomistic foundations of our understanding of mechanical and electronic properties of metallic materials in the frame work of dislocation theory and electron theory of metals finally shifted the focus of metallurgy to physics at the beginning of the 20th century. Eventually it engendered the discipline of metal physics, which has dominantly influenced the science of metals in the past 50 years. In fact, our current understanding of metallic and non-metallic materials on the basis of atomistic models has essentially been developed only in the past 80 years of research in metal physics. The objective of this research has been to describe the properties of a material on the basis of atomistic physical models, which can be formulated in terms of equations of state. This allows for a prediction of materials behavior on a theoretical basis and can be utilized to cut down on the costly and lengthy experimental investigations and testing of materials behavior.

In the sixties and seventies of the past century it became obvious that the urgent demand for high performance materials and competitive mass products had to include the development of non-metallic materials, for instance ceramics for high temperature components and plastics for a weight savings in automobiles and airplanes. Materials research revealed soon, however, that the foundations of physical metallurgy within limits can be readily applied to other materials, in particular to crystalline solids. Crystallography, constitution, diffusion, phase transformations, physical properties, and so on are the foundations of the understanding of all kinds of engineering materials.

Of course, there are also specific differences. For instance, dislocation theory which is indispensible for an understanding of plastic deformation of metals is of less importance for brittle ceramics, but it teaches the reasons for the brittleness and, therefore, offers respectives for counter actions. For polymers which are usually non-crystalline, an appropriate dislocation concept of their mechanical properties is still too complicated to be useful, and the deformation behavior of plastics is, therefore, currently restricted to phenomenological tribological models.

This development generated the strong belief that it is possible to derive a comprehensive description comprising the different classes of materials and that the future world be multi-material. This worldwide trend in the seventies of the past century caused the classical independent disciplines of metallurgy, ceramics, and plastics to merge to a new discipline "material science and engineering", encompasing both the science and engineering aspects of materials, and which has become our modern powerhouse of materials research and development.

1 Microstructure

When we buy a commercial product what we first note is its function and its appearence as, for example, the precious look of a noble metal, the engine of an automobile, the rope of a bridge, the wire of an electrical cable, the heat absorbing panes of a modern building, or the decorative ceramic and metallic parts of a modern bathroom. However, the usefulness of these items for their purpose and their life cycle will be determined by the properties of the material from which they were manufactured. Without any doubt we trust in the strength of the rope that suspends a large bridge, in the impact resistance of a ceramic hot plate in our kitchen or in the reliability of the little metallic buckets which provide the thrust of the turbine engine of an airplane at temperatures above 1000 °C. The properties of advanced materials are not so much affected by their overall chemical composition but rather by the specific arrangement of their constituents which we usually can not discriminate with our bare eye. The arrangement of the constituents of a material, i.e. the spatial distribution of elements, phases, orientations, and defects are subsumed under the term microstructure.

Castings or hot dip galvanized sheet reveal already to the bare eye that they are composed of small blocks that completely fill space. These blocks are referred to as grains or crystallites, if the nature of the material is crystalline, like metals, minerals or ceramics. Usually, however, the grain structure of a material is too small to be discerned by the bare eye. By careful surface treatment with grinding, polishing, and chemical etching the crystallites can be made visible under the optical microscope (Fig. 1.1). The corresponding image is referred to as a micrograph. Metallographic observation by optical microscopy is still an important stage of materials characterization and is referred to as optical metallography. The microstructure of the material as seen under the optical microscope is comprised of the grain structure of the material and its macroscopic chemically distinct phases.

The microstructure as revealed under the optical microscope is only a very rough characterization of the material. At higher magnification in the electron microscope it can be recognized that the macroscopically seemingly homoge-

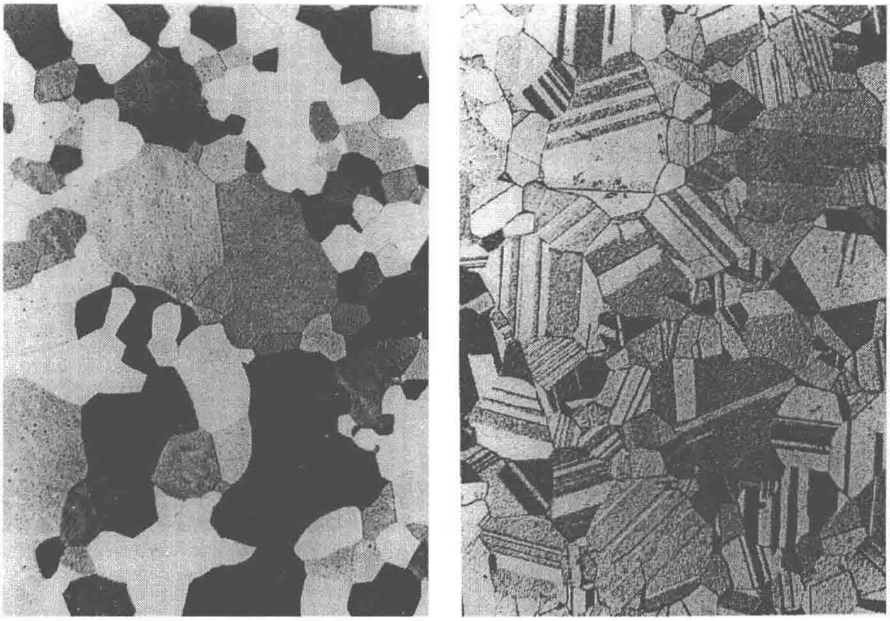

Fig. 1.1. Microstructure of recrystallized aluminium (a) and α-brass (b). The typical straight grain boundaries (twin boundaries) observed in brass are not present in aluminum and give the two structures a totally different appearance.

neous and perfect material itself contains a microstructure, i.e. microstructural defects, in particular dislocations (see Chapter 3), which are arranged in particular patterns, in addition to stacking faults, and, in most commercial materials, finely dispersed second phases (Fig. 1.2). Special materials also reveal additional microstructural elements, such as domain boundaries in magnetic materials, or antiphase boundaries in ordered solid solutions. The chemical composition can fluctuate over small distances as revealed by chemical microanalysis. Advanced materials can have a grain size in the submicrometer range (1 μm = 10^{-6}m) or even nanometer range (1 nm = 10^{-9}m) which can be resolved only under high magnification in the electron microscope. Therefore, imaging and chemical microanalysis in the electron microscope or with the electron probe microanalyzer have become standard techniques of modern metallography, i.e. advanced microstructural characterization.

Microstructural characterization is in itself interesting but becomes significant only in its relation to macroscopic properties and, therefore, requires a quantitative representation. The most fundamental microstructural information is the characteristic length scale, i.e. the grain size (grain diameter). One never, however, observes a uniform grain size, rather crystalline solids are composed of grains of different size, which is represented by the grain size dis-

Fig. 1.2. Microstructure of an engineering material (Al-alloy 2014), as it appears in an electron microscope image. Particles of a second phase and one dimensional crystal defects (dislocations) are visible. Also a grain boundary.

tribution. The characteristic value (1st moment, in the statistical sense) of the grain size distribution is the average grain size. Accurate values of grain size require advanced stereological methods. The most convenient and thus, most common is its derivation from optical micrographs, for instance by counting the intersections of grain boundaries with overlaid special geometrical curves in the micrograph, in the simplest case with a straight line or with spirals. Fortunately stereology proves that the average grain size obtained as the average intersection distance from a two dimensional micrograph also corresponds to the three dimensional average grain size within a factor of the order of one. More detailed information on the microstructure can be obtained from the grain size distribution. The grain size distribution function is defined as the statistical frequency of a specific grain size. Evidently, a mathematically exact given grain size may not exist, therefore, it is common and reasonable to count the frequency of grains with sizes that fall within a predefined grain size interval. For instance, all grains with a grain size between 0 and 10 μm, from 10 to 20 μm, and so on, are summed up. The representation of the frequency of a particular characteristic based on intervals of a measurable feature is referred to as histogram (Fig. 1.3).

A measured histogram of the grain size distribution is not symmetrical with regard to the average value, i.e. the most frequent value (median value) or the grain size D_m where the grain size distribution has its maximum, is