

Preface

Most current studies tend to present the knowledge on interfaces in crystalline materials by simultaneously considering homophase interfaces or grain boundaries, and hetero-interfaces located either between two crystals of the same material but with two different structures (such as ferrite/austenite in steels), or between two different materials (metal A/metal B, metal oxide, metal–semiconductor). In this work, we deliberately choose to limit our presentation to grain boundaries. Despite the fact that the crystals on both sides of the interface display the same structure and the same composition, these interfaces are not simple. Numerous questions about their structures, their defects, and their organizations in the material still have to be solved. In each chapter, we aim to highlight these questions after having selected well-established data. In particular, we underline the difficulties in going from an ideal grain boundary (akin to a perfect crystal) to a real grain boundary (analogous to a crystal with defects). Subsequently we address the difficulties in going from an isolated grain boundary in a bicrystal to that included in a polycrystal grain boundary network, where each grain boundary is constrained at triple junctions.

Two main ideas prevail in the concept of this work. The first idea is implicitly contained in the book sub-title *From Theory to Engineering*: to know in order to control and even improve. In this perspective, we not only approach the grain boundaries at the current time, but we also try to look into the future of grain boundary research and applications. The underlying question is the grain boundary contribution to the overall material properties, the improvement of which being the final goal in materials science. Now, at the beginning of the twenty-first century, grain boundary engineering, the dream of the 1980s, seems to be taking shape on the horizon. Indeed, with the development of new experimental and computational techniques, progress has been made which enables us to fill the gap between the scales and to move backward and forward between the world of atoms and that of objects. For this reason, the present work is not restricted to a state-of-the-art report, but it moves toward engineering by considering the exchanges between a grain boundary and the other crystalline defects and, moreover, by immersing the boundary in a *practical* environment, i.e. connected with other grain boundaries.

The second idea, strongly associated to the previous one, reveals a constant effort to overcome the dichotomy between the “whole” and the “parts”. It can be summarized as: *from the individual to the collective* or *from the element to the whole*. And again, the objective is to gain a better understanding and an awareness of the practical applications.

In engineering, not only the responses of individual grain boundaries to various stimuli, but also the collective behavior of a grain boundary network must be known. However, grain boundary properties are not explicitly considered in this book for the following reasons. The basic mechanisms at grain boundaries are similar to those occurring in the crystal in several cases such as diffusion and plastic deformation. The reader may find information in specific books dedicated to these properties (references are given at the end of the book). Although the behavior of isolated grain boundaries has been studied extensively, no agreement exists on the elementary processes in cases of migration, corrosion, and wetting. Furthermore, very little is known concerning the grain boundary electric and magnetic properties. Generally, the properties vary with the grain boundary geometry. However, apart from the coherent twins that display very particular behaviors, ambiguities remain about the specific behaviors of other grain boundaries. Most often, the grain boundary chemistry erases the particularities linked to the geometry. In numerous experiments, the difficulty to evaluate the solute content in the intergranular region leads to contradictory results for a same stimulus, a same material, and a same type of grain boundary. The main reason to postpone the consideration of grain boundary properties is the lack of data on the collective grain boundary behaviors in polycrystals. However, the situation could progressively evolve with the simulation of local grain boundary textures and by the percolation approaches of the grain boundary ensemble. Finally, although not treated explicitly in a separate chapter, grain boundary properties are certainly treated implicitly. The mechanical behavior may be understood on the basis of the interactions between lattice dislocations and grain boundaries and of the intergranular stress relaxation under the effects of temperature and time. Other approaches of grain boundary network properties are also briefly stipulated.

The examples treated in this book concern different crystalline materials: metals, ceramics, semiconductors, and superconductors. In earlier times, grain boundary studies mainly developed in the field of metallurgy. Conceptual advances were obtained from high-resolution transmission electron microscopy observations of semiconductor bicrystals. Only the results of experiments and simulations are given in this volume. For the understanding of the electron microscopy images and of the calculated grain boundary structures, the reader may refer to the general references given at the end of the book, which also include books dedicated to grain boundaries and to certain properties often mentioned. Specific references are given at the end of each part and may be repeated from one chapter to the other.

Going *From Theory to Engineering*, three stages need to be passed, constituting the three parts of the book.

Part I deals with the concept of a *perfect grain boundary*, at equilibrium, and questions the maintenance of its crystalline state. The notions of order and disorder always raise questions from a philosophical point of view. *Beauty* is traditionally linked to order and science cannot escape this esthetic connotation. Working on a beautiful object is a noble task. For several years, studies in the grain boundary domain mainly concern grain boundaries that possess symmetry and purity. *Noble* tools such as transmission electron microscopy and atomistic simulations were used to improve understanding of grain boundary order. At the other end of this hierarchy of the beauty, there are ugly and impure grain boundaries, their proportion in polycrystals generally being high. They play a major role in the material properties. This first part presents the notion of *bicrystallography*, followed by the description of grain boundaries in terms of dislocations and in terms of structural units of atoms, with a special focus on the limits of these descriptions. The reasons for which a grain boundary adopts a given structure are also discussed, knowing that order and energy are not necessarily linked.

Part II brings us to the *faulted grain boundary*. It attempts to reveal the influence of the grain boundary structure on its defects, their formation, and their accommodation. Point, line, and volume defects are considered. Interstitial and substitutional solutes in excess in a grain boundary, resulting from a *segregation* phenomenon, strongly change the grain boundary behaviors. They may lead to pre-wetting accompanied by an important widening of the grain boundary region that possibly becomes non-crystalline. In the presence of segregated elements, the differences due to geometrical parameters may be obscured. Segregation may be the origin of the preferential formation of a second phase at grain boundaries that notoriously affects intergranular corrosion, migration, and deformation. Precipitation at grain boundaries and 3D defects well deserve to be analysed in this part. Finally, the interactions between boundaries and lattice dislocations yield strong disturbances at grain boundaries. The elementary mechanisms for the entrance of dislocations in a grain boundary and for the relaxation of the associated intergranular stresses are discussed in greater detail in this part. They constitute the necessary support to allow a good understanding of the mechanical properties of isolated grain boundaries, and subsequently for grain boundaries included in an ensemble.

Part III of the book is specifically devoted to these *grain boundary ensembles* starting from the *triple junction* to real grain boundary networks in polycrystals. To our knowledge, this is the first monograph to sum up the different approaches that have been developed in recent years in an engineering direction. Despite reserves, we take risks to select some mesoscopic and macroscopic studies of grain boundaries that contribute to a better understanding of the grain boundary network configuration in a material. It is an attempt to combine our knowledge of the part and of the whole, aware that there is still a huge territory to explore. In particular, general grain boundaries remain largely unknown. Furthermore, grain boundaries spatially confined in nanocrystals confer specific properties to the material. They also seem to escape order. With the development of Chaos theory, these disordered objects give rise to new interest. Generally, though, the scientific attitude in the

field of grain boundaries remains *classical*: it deals with the research of an hindered order behind an apparent disorder. The approaches developed in that domain are beyond the scope of the deterministic disorder.

The book is addressed to graduate students preparing a thesis, to engineers and to researchers in materials science; it attempts to give basic notions on grain boundaries and to give rise to research subjects in that field. It also tries to interest the scientific community in a major component of the material microstructure, the importance of which increasing as the grain size decreases. This constitutes a real challenge with the development of nanomaterials.

It is my sincere hope and final goal that the knowledge presented and the ideas developed in this work may help future researches on grain boundaries.



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Grain Boundaries

From Theory to Engineering

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