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First Principles Modelling of Shape Memory Alloys

Molecular Dynamics Simulations

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Preface

The fascinating properties of shape memory alloys have inspired engineers ever since their discovery some 60 years ago. The reason for their attractiveness lies in the fact that these materials combine both functional and structural properties. They share their processing techniques with metals, can be cast or sintered into any shape and they can be rolled, cut, milled and welded. They are progressively ductile and are electrically and thermally conductive. Thus, their physical properties admit structural functionality. What makes them special is the fact that all these properties strongly depend on temperature. One consequence of this dependency yields the characteristic shape-memory effect: shape memory alloys can recover processed reference configurations after significant plastic deformations simply upon a change of temperature, thus adding functional abilities to structural elements. The epithet *smart material* was swiftly coined.

This work deals with a theoretical investigation of this class of alloys at the atomic scale. Here, we are concerned with length and timescales some orders of magnitudes below typical current engineering applications. One might object that these scales were not within the realm of an engineering faculty, where the majority of work deals with the design of useful technical applications. A 3-fold reply might be given to this objection: based on the historical context, with regard to the subjects contents and due to the need for interdisciplinary research work.

Historically, material sciences emerged at the intersection of engineering demands and scholastic nature sciences. Even before the theory of the atomic structure of matter was gradually formulated in the nineteenth century, natural philosophers like Descartes speculated about a microscopic conception of matter. However, techniques first needed to be developed before experimental evidence was obtained.

Milestones in the development of the materials sciences were set by the engineers, Osmond and Martens, who brilliantly advanced the microstructural characterisation of steel. Since their days, all improvements in microscopy directly

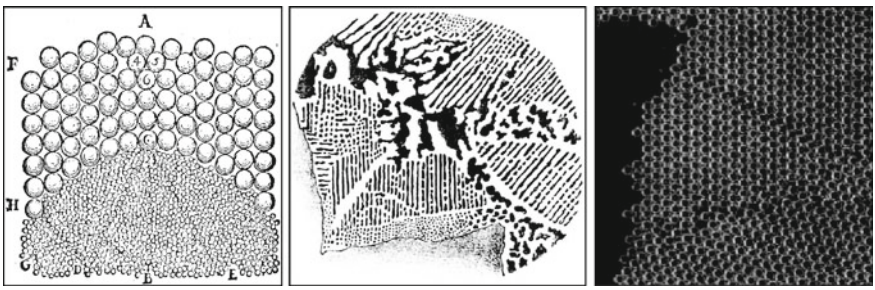

Fig. 1 Approaches to the microstructure. 1644: Descartes speculates about the particulate character of matter [1]. 1878: Martens draws micrographic images of etched steel [2]. 1947: Bragg and Nye model close-packed lattices by bubble rafts on soap suds [3].

affected the understanding of materials; from light microscopy down to the atomic level by transmission electron microscopy. However, microscopy today can still not reveal how the observed structures evolve *dynamically*. Here, molecular dynamics (MD) simulations may assist with regard to this: From first principles—Newton's Equations of Motion—we can dynamically simulate nucleation and growth of microstructural forming processes in solids on a computer. Hence, lattice transformations can be observed and analysed in situ rather than post mortem. In MD, some macroscopic variables can be controlled (temperature, applied load, etc.) during which the reaction of the test system is studied. Owing to this similarity to "real-world" laboratory experiments, the term "MD simulations experiments" is frequently used. Nota bene, even a method such as this has an analogous precursor: In 1947, Bragg and Nye investigated bubble rafts on soap suds as a dynamic model for domain structures and dislocations in close-packed lattices. Their intuitive images soon became part of the textbook literature. The bubble model also teaches us that a comprehensive model must not necessarily be complicated if it only represents the fundamental physics correctly. In this case, even simple models may contribute new insights into the subject matter under investigation and widen the scientific horizon.

In general, applications currently demand miniaturised designs. This tendency has, during the last two decades, already borne a new branch of engineering, the so-called nanoscale technology. Here, applications are particularly restricted by their weight and size, therefore a combination of the structural and functional features make shape memory alloys attractive as actuators or propulsion elements. Thin film applications processed, for example, by sputter deposition techniques, truly range in nanoscale dimensions and thus, in principle, become accessible to atomistic modelling. Also, atomistic methods can serve to determine local or boundary conditions for continuum-scale models. The necessary mathematical

techniques needed to bridge the gap between the atomic up to the continuum scale have already been developed (coarse-graining methods) and have been applied to, for example, cracktip simulations.

The last item concerns the need for interdisciplinary research work. Contemporary solid-state physics focuses on the subatomic structure of metals, hence addressing length and timescales far below the atomic level. Here, for example, ab-initio calculations based on quantum mechanics improve our understanding of the energetic states which determine the cohesive forces between atoms in lattices. With the increasing availability of computational resources, these methods quickly became more popular and readily spawned a lively research community. In principle, such methods can be used to derive the interaction potentials needed by the MD method. Therefore, MD again represents a scale bridging technique which is able to link subatomic modelling to the mesoscopic microstructural calculations under consideration in materials sciences. It is prudent to maintain this link: in order to further interdisciplinary research as well as to share results and discoveries between the disciplines. From a broader perspective, this topic also addresses didactic issues.

With this background in mind, the reader is now warmly welcome to share some endeavours towards a better understanding of shape memory alloys on the atomic level. The core of this work deals with a two-dimensional (2D) Lennard-Jones model, which will be proven to represent a reliable model system for martensite/austenite transformations. We present MD simulations of martensitic phase transformations, studying post-transformation microstructures and motile austenite-martensite interfaces. The material model exhibits full thermo-mechanical coupling and is thus capable of related material behaviour such as pseudo-plasticity/elasticity and the shape memory effect. Even in 2D, rich transformation morphologies can be studied which exhibit striking similarities to real materials.

Among the observed phenomena, we discuss the nucleation and show the propagation of motile transformation fronts, martensitic plate growth, the twinning process, the formation/accommodation of martensitic domain structures, the generation of transformation-related lattice defects and their influence on the transformation processes. The evolution of defect structures is investigated by means of simulations of cyclic transformation/reverse transformation processes. During transformations, lattice defects are generated which affect subsequent transformations and vary the potential energy landscape of the sample. Some of the defects persist through the transformation, providing nucleation centres for subsequent cycles. Such defects may provide a memory of previous structures, and thereby may be the basis of a reversible shape memory effect.

Much effort was spent in describing the simulations as complete as possible using words and figures. For technical reasons, some colour figures are converted into greyscale in the printable version of this book. The respective colour figures are available in the online version. In addition to these, we have attached videos

which afford an intuitive understanding of the processes discussed. These videos are available online at www.olli-kastner.de/pub/md.

Acknowledgments

The work presented here evolved over a 4 year period at the Department of Materials Science, Institute for Materials of the Ruhr-University Bochum, Germany. My thanks are due to the Director of this chair, Gunther Eggeler who, in 2005, gave me the marvellous opportunity to participate in his research group on shape memory materials. A substantial basis for my work was certainly Gunther Eggerler's generous and remarkable technical support. Moreover, and even more importantly from the perspective of an un-established postdoctoral fellow, was his intellectual backing and his complete trust in the ongoing research activities. All this provided the creative and autonomous research conditions I very much appreciated.

At ESOMAT 2006, I received the opportunity to communicate some preliminary results of my research model to Graeme Ackland who, by that time, was already an internationally honoured scientist in this field. Luckily, the model convinced him and we started a collaboration which frequently took me to his department at the University of Edinburgh. The present work gained much persuasiveness and conciseness by Graeme Ackland's experience, extraordinary knowledge and intellectual brilliance. I thankfully appreciate his contributions.

The work also improved thanks to continuous considerations by many colleagues in the course of seminars and conferences, by visiting guests and during peer reviews. Special thanks are due to Wolf Weiss (Weierstrass Institute for Applied Maths, Berlin/Germany), Roni Shneck (Ben Gurion University of the Negev, Beer-Sheva/Israel), Stefan Seelecke (Universität Saarbrücken/Germany), Yonzhong Huo (Fudan University, Shanghai/China) and to my colleagues at the Ruhr-University Bochum.

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