Polycrystals: Microstructure and Effective Properties Workshop

Monday 26 March 2018

Variant coupling of martensite and bainite structures in steels

Goro Miyamoto (Tohoku University)

Lath martensite and upper bainite in steels consists of complicated hierarchical structure, such as packet, block and lath structures, resulted from multiple variants of specific orientation relationship with respect to parent austenite. Since those boundaries, except lath boundaries, are separated by different variants and impede deformation and/or fracture, characterization of variant structure is of a great importance in order to clarify relationship between microstructure and mechanical properties. The present authors have quantified variant pairing tendency in lath martensite and bainite structures on a basis of EBSD measurement and have revealed that different variant coupling appears depending on composition or transformation temperature. The preferential variant pairs observed are in twin-related or to share the same Bain correspondence or the same close-packed plane parallel relation. In the presentation, the reason of coupling of specific variants is discussed from the viewpoints of strain continuity at variant boundary (Kinematic Compatibility condition) and reduction of average strain (self-accommodation).

Mechanistic Models of Deformation Twinning and Martensitic Transformations

R. C. Pond (College of Engineering, Mathematics and Physical Sciences, University of Exeter)

The geometrical theory of deformation twinning (DT) is based on the notion of an invariant plane (IP), and the phenomenological theory of martensite crystallography (PTMC) is an adaptation of this. While the mechanistic model of DT, based on the concept of a twinning dislocation gliding conservatively along a low-energy interface, was initiated over 70 years ago, its adaptation to martensitic transformations has only been developed more recently. In this presentation, geometrical and mechanistic approaches are compared and contrasted: experimental observations underpinning the mechanistic model are presented.

The dislocation model of type I and compound twinning has been verified experimentally, and is consistent with the geometrical theory. Contrarily, experimental studies do not confirm that type II twins form by the same mechanism. A new model of type II twinning is presented wherein twinning dislocations are generated on the conjugate plane, and accumulate to form a tilt wall: accommodational relaxation of such walls requires partitioning of the rotational distortions between the adjacent crystals, thereby forming the type II habit. While the overall deformation produced by this mechanism is consistent with the geometrical theory, the mechanism of formation of type I and compound twins (glide twinning} is different from that for type II twins (glide/rotation twinning).

European Research Council
Established by the European Commission

UNIVERSITY OF OXFORD

The mechanistic model of martensitic transformations parallels that for twinning. In general, no IP exists between distinct phases, but low-energy epitaxial interfaces do arise. These generally require two sets of line-defects to accommodate misfit: one set is slip or twinning (as in the PTMC), and the other is an array of glissile transformation dislocations. Synchronous motion of the latter along the interface produces the displacive transformation, and experimental observations support this model. Predicted magnitudes of transformation shear and misorientation using this model are the same PTMC values, but habit planes differ, slightly in most cases. This discrepancy arises because long-range strain is removed by the defect array in the equilibrium interface, but the attendant rotational distortions are partitioned between the phases in a manner dependent on their relative elastic properties.

Microstructures in SMA: Rigidity, Non-Rigidity and Simulations

Angkana Rüland (Max Planck, Leipzig)

In this talk I will discuss a striking dichotomy which occurs in the mathematical analysis of microstructures in shape-memory alloys: On the one hand, some models for these materials display a very rigid structure with only very specific microstructures, if one assumes that surface energies are penalised. On the other hand, without this penalisation, for the same models a plethora of very wild solutions exists. Motivated by this observation, we seek to further understand and analyse the underlying mechanisms. By discussing a two-dimensional toy model and by constructing explicit solutions, we show that adding only little regularity to the model does not suffice to exclude the wild solutions. We illustrate these constructions by presenting numerical simulations of them. The talk is based on joint work with J. M. Taylor, Ch. Zillinger and B. Zwicknagl.

High Angular Resolution Electron Backscatter Diffraction studies of Fe-C Martensitic Steels

Tomohito Tanaka and Angus J Wilkinson (Department of Materials, University of Oxford)

Steels are a vastly adaptable class of materials offering an incredible range of engineering properties brought about through sophisticated manipulation of microstructure. Lath and plate martensite structures formed in low- to medium-carbon steels are of particular industrial significance. Martensitic phase transformation from the high temperature face centre cubic austenite to the body centre tetragonal martensite leads to a complex hierarchical microstructure which balances lattice strain and interfacial contributions to energy. As the carbon content is increased X-ray diffraction studies have shown that the average c/a ratio of the martensite increases, while microscopy shows a refinement in microstructural lengthscale. There is, however, a lack of knowledge concerning the microscopic variation in tetragonality. We address this knowledge gap using some careful measurements using high resolution electron backscatter diffraction (HR-EBSD).

Polycrystals: Microstructure and Effective Properties Workshop

Several Fe-C martensitic steels were austenitised and water-quenched followed by liquid nitrogen cooling and then metallographically prepared for EBSD analysis. A small (10x10x1 μm^3) well-annealed interstitial free (IF) steel sample was mounted on each martensite block. Theoretical EBSD simulations generated using dynamical diffraction were matched to experimental EBSD patterns from the IF steel to give an accurate determination of the detector geometry. Pattern matching between EBSD from the martensitic steels and simulations conducted for BCT crystals at different c/a ratios were then used to determine the tetragonality at a few local points on the sample (fig. 1). We then employed the HR-EBSD approach which uses cross-correlation at many sub-regions across the EBSD patterns is used to determine pattern shifts relative to some reference/seed patterns. Using the HR-EBSD mapping from the reference/seed points at which the detailed pattern matching measurements had been made allows more complete mapping of the tetragonality variation within the microstructure to be constructed (fig. 2).

Fig. 1: Point analysis

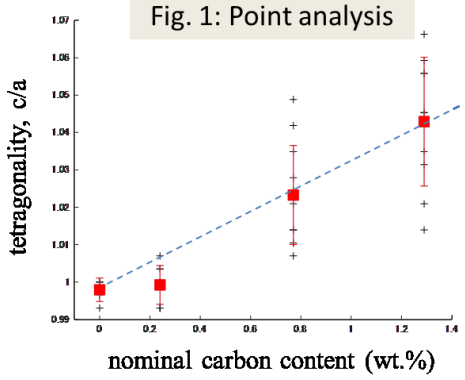
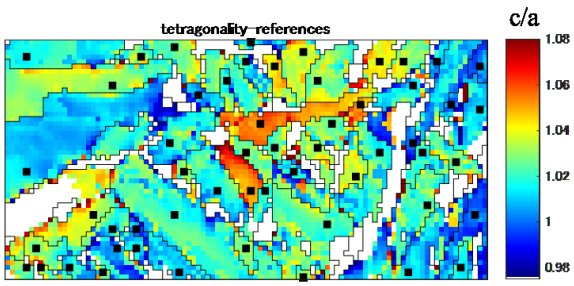


Fig. 2: Map analysis



Tuesday 27 March 2018

Martensitic microstructure in nanocrystalline NiTi shape memory alloys - experiments & modelling

M. Petersmann1, T. Antretter1, F.D. Fischer1, C. Gammer2, T. Waitz3

1) Institute of Mechanics, Montanuniversitaet Leoben, Franz-Josef-Straße 18, 8700, Leoben, Austria
2) Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstrasse 12, Leoben 8700, Austria
3) Physics of Nanostructured Materials, Faculty of Physics, University of Vienna, Boltzmangasse 5, 1090 Vienna, Austria

In nanocrystalline NiTi, the microstructure of compound twinned variants of the B19´monoclinic martensite is analysed at an atomic scale using high-resolution transmission electron microscopy. A model for these laminated nanostructures is set up, combining classical energy minimization with finite element calculations in a computationally fully automated manner. The crystallographic model considers the complete set of anisotropic elastic constants to elucidate the interaction of

martensite in adjacent grains via self-accommodation of their transformation strains. The sequence of grains subjected to transformation as well as the selection of martensitic variants within the grains is obtained yielding the evolution of the total interface energy as well as the strain energy, dominating our approach.

A model for polycrystalline shape-memory alloys derived from microscopically motivated assumptions

Barbora Benešová (University of Würzburg)

Shape-memory alloys feature a complicated rheology at the single crystal level with a number of energy wells leading to fine microstructure of strain states. On the other hand, when looking only at effective material properties at the polycrystalline level, it is customary to use more phenomenological models that do not inherit much from the single-crystal. In this talk I would like to present a derivation of a model for polycrystalline shape-memory alloys built up upon the idea that martensite transforms to austenite only via a specific structure of martensite called ""transformation favourable martensite"". This seems to a possibility on how to implement some qualitative knowledge of the behavior on the single crystalline level into phenomenological modelling that allows for a sound mathematical analysis and finite-element computations. Indeed, the model is rate-independent and embedded into the framework of general standard materials making it automatically thermodynamically consistent. Moreover, it allows us to construct a so-called energetic solution, which I will also show in the talk. This has the advantage that a straightforward discretization of the model, that can be used in finite-element computations, is readily available.

This is joint work with M.Frost and P. Sedlák (both Prague).

Hydrogen-related fracture behavior of martensitic steels

Akinobu SHIBATA Department of Materials Science and Engineering, Kyoto University

It is well known that the presence of hydrogen leads to catastrophic and premature fracture in metals and alloys. This phenomenon is termed ‘hydrogen embrittlement’, ‘hydrogen-related fracture’, ‘delayed fracture’, etc. Several models have been proposed to account for hydrogen-related fracture. However, the underlying mechanism for hydrogen-related fracture is not fully understood. From recent economic and environmental viewpoints, demands for high-strength steels are increasing more and more. Because susceptibility to hydrogen embrittlement increases with the increase of the strength of materials, hydrogen embrittlement is now becoming a major concern of steel society. The present talk introduces our recent research on the microstructural / crystallographic features and propagation process of hydrogen-related fracture in martensitic steels.

The martensite structures with relatively low strength exhibited quasi-cleavage fracture. Crystallographic orientation analysis demonstrated that the quasi-cleavage fracture occurred on {011} planes. On the other hand, the macroscopic fracture surface morphologies of the martensite structures with relatively high strength appeared to be intergranular-like. However, nature of the fracture was somewhat different from a typical intergranular fracture, and the fracture surfaces consisted of facets parallel to {011} planes on a microscopic level. The experimental results strongly suggest that the crystallographic feature of {011} plane itself has an important role on the hydrogen-related fracture. The reconstructed fracture propagation process by fracture surface topography analysis (FRASTA) suggested that the fracture propagation path changed with the proceeding fracture; the intergranular fracture occurred and propagated suddenly at the early stages of fracture, and then the quasi-cleavage fracture gradually propagated. In addition, crack formation mechanism was discussed from the viewpoint of microstructure, hydrogen accumulation behavior, and local stress / strain distribution.

On the characterisation of subclasses of symmetric polyconvex functions

Anja Schlömerkemper (University of Würzburg)

The notion of symmetric quasiconvexity plays a key role for energy minimization in the setting of geometrically linear elasticity theory. Due to the complexity of the former, a common approach is to retreat to necessary and sufficient conditions that are easier to handle. The focus of this work lies on symmetric polyconvex functions and the characterisation of relevant subclasses in the two- and three-dimensional setting. In particular, we provide an example of a symmetric rank-one convex quadratic form in 3d that is not symmetric polyconvex. The construction is inspired by the famous work of Serre in the non-symmetric context. Despite their theoretical interest, these findings may turn out useful for computational homogenisation and relaxation.

This is joint work with Omar Boussaid (University of Chlef) and Carolin Kreisbeck (University of Utrecht)."

Energy bounds and estimates for polycrystalline shape memory alloys at small strains

Michaël Peigney (École des Ponts Paris Tech)

Adopting the framework of nonlinear elasticity at small strains (geometrically linear setting), the mesoscopic energy of a monocrystalline shape memory alloy is obtained as the quasiconvex enveloppe of a multi-well, piecewise quadratic function. Assuming a large separation between the length scale of the martensitic microstructures and the length scale of the grains, the effective energy of a polycrystal is obtained by homogenization, viewing groups of grains with the same orientation as homogeneous materials governed by mesoscopic energy function. Except in few special cases, exact expressions of the effective energy remain elusive.

In this talk, much emphasis is put on lower bounds (on the effective energy) that can be obtained by combining the translation method (Milton, 1990 ; Pipkin, 1991) with a Talbot-Willis (1985) type formulation for taking some statistical information on the polycrystalline texture into account. The resulting bounds incorporate both intra-grain compatibility conditions and inter-grain constraints.

To get some insight into the behavior of those bounds, we first consider a simple example for which explicit expressions can be obtained. The issue of calculating the bounds for more complex polycrystals is addressed. In more detail, we present a numerical strategy for evaluating the bounds in a computationally efficient manner. Some results are obtained for representative examples of textures (such as rolled textures in NiTi sheets).

Numerical and experimental evidence suggest that the obtained lower bounds may significantly underestimate the effective energy in some cases. Building on the mathematical formulation of lower bound, we introduce an estimate that may be closer to the effective energy while still satisfying known bounds.

Wednesday 28 March 2018

Micromechanical modeling of polycrystalline shape memory alloys - energies and evolution

K. Hackl, R. Fechte-Heinen, P. Junker, J. Waimann (Ruhr-Universität Bochum, Germany)

Shape memory alloys can be described in a uniform way relying on energetic considerations only. We present a micromechanically motivated model for polycrystalline shape memory alloys. The approach is based on energy minimization and includes hysteresis effects via various formulations of dissipation potentials. It is capable of reproducing most important aspects of the material behavior such as pseudoelasticity, pseudoplasticity and shape memory effect. Special attention is given to the aspects of experimental validation and parameter identification which demonstrate nicely the full potential of variational methods.

[1] S. Govindjee, K. Hackl and R. Heinen. "An upper bound to the free energy ofmixing by twin-compatible lamination for n-variant martensitic phase transformations.: Continuum Mech. Thermodyn., 18, 443, 2007.

[2] K. Hackl and R. Heinen. "An upper bound to the free energy of n-variant polycrystalline shape memory alloys." J. Mech. Phys. Solids, 56, 2832, 2008.

[3] K. Hackl and R. Heinen. "A micromechanical model for pretextured polycrystalline shape-memory alloys including elastic anisotropy." Continuum Mech. Thermodyn., 19, 8, 2008.

[4] P. Junker and K. Hackl. "A novel approach to representative orientation distribution functions for modeling and simulation of polycrystalline shape memory alloys." Int. J. Numer. Meth. Eng. 98 (11):799-818, 2014.

[5] P. Junker, S. Jaeger, O. Kastner, G. Eggeler and K. Hackl. "Variational prediction of the mechanical behavior of shape memory alloys based on thermal experiments." J. Mech. Phys. Solids 80:86-102, 2015.

[6] J. Waimann, P. Junker and K. Hackl. "A coupled dissipation functional for modeling the functional fatigue in polycrystalline shape memory alloys." European Journal of Mechanics-A/Solids. 55:110-121, 2016.

Experimental study and phenomenological modeling of NiTi SMA

Petr Sedlak (Institute of Thermomechanics, CAS, Prague)

Collaborative work with: M. Frost, H. Seiner (Institute of Thermomechanics, CAS, Prague), P. Sittner, L. Heller, P. Sedmak (Institute of Physics, CAS, Prague), B. Benesova (University of Würzburg)

In this presentation, both experimental results and simulations based on phenomenological modeling will be presented, focusing on three aspects of the behavior of polycrystalline NiTi shape memory alloys:

1) An extensive experimental study of mechanical behavior of NiTi wires under combined tension-torsion loading revealed complex mechanical response associated with simultaneous occurrence of two dissipative inelastic mechanisms - martensitic phase transformation and martensite reorientation. The intention to formulate a mathematically consistent model capturing experimental observations led to formulation of a proper dissipation function, which controls mutual interplay of both dissipative mechanisms in the model formulated within the framework of generalized standard solids [1]. Several comparisons of experimental and computed results verified plausibility of the proposed function although its derivation assumed a virtual intermediate zero-strain martensitic state during formation of stress-induced martensite, which has no counterpart on single crystal level.

2) In particular geometries and loading modes, martensitic phase transformation develops inhomogenously, in a highly localized manner. We have analyzed morphology and mechanics of a macroscopic transformation front separating regions of austenite and martensite phases in a particular case of NiTi superelastic wire under tension. Three-dimensional X-ray diffraction method (3D-XRD) was employed to determine complete strain and stress states of polycrystalline grains close to the transformation front [2]. Taking into account the experimental findings, we adapted our macroscopic constitutive model of NiTi by modifying the internal interaction energy term and including non-local (gradient-like) effects. Good agreement between simulations and the

experiment was achieved in this particular case, but generalization for different loading modes is not obvious.

3) Behavior of polycrystalline NiTi beyond the strain recoverability limits (at high stresses or high temperatures) is characterized by simultaneous evolution of martensitic transformation and irreversible plastic deformation [3]. In agreement with theoretical predictions based on the mathematical theory of martensitic microstructures and the crystal plasticity theory, we have observed strong transformation-plasticity coupling only during the reverse martensitic transformation in experiments. Moreover, the plastic deformation in NiTi originated primarily from deformation twinning in the B19' martensite and not form the dislocation slip in austenite. A new TRIP mechanism, which is mainly temperature-driven, was suggested to capture the evolution of the plastic deformation.

[1] Sedlak, P., Frost, M., Benesova, B., Ben Zineb, T., Sittner, P., Thermomechanical model for NiTi-based shape memory alloys including R-phase and material anisotropy under multi-axial loadings, Int. J. Plast., Vol. 39 (2012), pp. 132-151.

[2] P. Sedmák, J. Pilch, L.Heller, J. Kopeček, J. Wright, P. Sedlák, M. Frost, P. Šittner, Grain-resolved analysis of localized deformation in nickel-titanium wire under tensile load, Science 353 (2016), 559-562.

[3] P. Šittner, P. Sedlák, H. Seiner, P. Sedmák, J. Pilcha, R. Delville, L. Heller, L. Kadeřávek, On the coupling between martensitic transformation and plasticity in NiTi: experiments and continuum based modelling, Progress in Materials Science, under review.

Polydomain liquid crystal elastomers

Kaushik Bhattacharya (Caltech)

Liquid crystal elastomers are rubbery solids with liquid crystal mesogens incorporated into their main chains. They display an isotropic to nematic phase transformation accompanied by a large spontaneous deformation. Depending on how these liquid crystal elastomers are synthesized, they can either be a mono domain (uniform liquid crystal order) or polydomain (nonuniform liquid crystal order). This talk will describe various phenomena and mathematical questions related to the effective behavior of polydomain liquid crystal elastomers.
