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Book of Abstracts

Microstructure formation in titanium alloys and correlated mechanical properties.

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The studies on titanium alloys developed since several years in our group aim to understand the mechanisms of formation of these microstructures, considering several alloys with different chemical compositions, the effect of thermal treatment and the relationships between microstructure and mechanical properties. In addition, modelling approaches of the transformation kinetics, the microstructure formation are/were developed in order to be able to calculate the transformation kinetics and morphologic features whatever the chemical composition (given a selected range of composition).
The presentation will focus on the main characteristics of microstructure formation in titanium alloys depending on the thermal treatments applied to the material. The morphology of the precipitated phase, its chemical composition will be linked with the transformation mechanisms. In addition to the microstructure/morphology of the precipitated phase, microtexture formation will be considered and the role of elasticity will be emphasized. Finally, the link between microstructure and mechanical properties will be illustrated.

Modeling of solid-state phase transformations in metallic alloys

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First, I will show rapidly a few examples of recent achievements in modeling phase transformations with a particular emphasis on their interactions with elasticity and plasticity handled with phase field models. Then, I will move to recent advances in the modeling of phase transformations in beta-metastable Ti alloys, in connection with the large set of experiments peformed in the research group of Pr. Elisabeth Aeby-Gautier. For that purpose, I will start with a physically-based nucleation-growth model at the mm scale designed to compute the kinetic diagrams and relying on the Calphad approach to handle multicomponent alloys, and discuss different issues remaining opened which require models at lower scales. Questions related to the colonies of Widmanstatten alpha plates will first be adressed using phase field calculations. In particular, I will show that their growth direction and kinetics are essentially determined by the anisotropy of elastic energy generated by the eigenstrain associated with the bcc to hcp transformation. Then, I will address the influence of elasticity on the nucleation and growth of intragranular alpha"/alpha precipitates featuring specific spatial patterns. Finally, I will discuss the possible role of omega precipitation on the nucleation of alpha".

Effect of thermal path on the precipitation sequences in beta metastable titanium alloy

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Understanding and further modeling of microstructure formation, i.e. transformation sequences and kinetics need in situ characterization to quantify the transformation kinetics as well as to get additional characteristic for the multiphase polycrystalline component. In situ characterization using high energy X-ray diffraction (ID15 ESRF) were realized in parallel to more conventional techniques (electrical resistivity measurement or TEM observation) to characterize transformations in beta metastable titanium alloy. High energy X-ray diffraction allowed to analyze a consequent volume of the specimen, avoiding surface effects, and to increase the sensitivity and acquisition frequency for the diffraction patterns.

The influence of the thermal path on the transformation sequences will be shown. Notably, we will illustrate the formation of different metastable states for precipitation during ageing. A complex sequence occurred depending on the heating conditions. For some lower heating rate, hexagonal isothermal omega precipitate formed at first. Increasing the time or temperature, an orthorhombic phase (alpha”) appeared before the transformation into the alpha phase while peaks corresponding to omega vanished. It is worth mentioning that HEXRD clearly demonstrated the formation of a metastable orthorhombic phase that is never mentioned in TEM observations. The transformation sequences clearly influence the final microstructure and the resulting mechanical properties.

ω phase particles in Ti alloys studied by small-angle x-ray scattering

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Metastable β titanium alloys contain a sufficient amount of alloying elements which suppress the transition from a body-centered cubic β phase (thermodynamically stable at high temperatures) to a hexagonal close-packed α phase (stable at low temperatures). In a certain concentration range of the β stabilizing elements, particles of metastable ω phase form in the metastable β titanium alloys. The ω phase particles are a few tens of nanometers in size and are homogeneously distributed throughout the β matrix. They have a hexagonal structure and are coherent with the β phase. Due to these facts, ω particles have a significant impact on further phase transformations in the alloy and on its mechanical properties.

In this research, ω phase particles and their evolution during ageing were studied by small-angle x-ray scattering (SAXS). SAXS measurements were done on single-crystalline material prepared in an optical floating zone furnace. The analysis of SAXS measurements showed that the ω particles are weakly ordered in a cubic "superlattice" aligned along $<100>_\beta$ directions of the bcc β phase. From *in situ* SAXS experiments carried out during isothermal ageing, the concentration profile around growing ω phase particles was determined using a diffusion equation with moving boundary conditions. The evolution of ω particle sizes and distances was also determined. Moreover, the diffusion coefficient of the alloying elements as well as the activation energy of ω particles growth were evaluated.

Parametric Model of Evolving Dislocation Curves in Persistent Slip Band Under Stress/Strain Controlled Regimes

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ABSTRACT

A standard tool in an investigation of deformation microstructure has become the Discrete Dislocation Dynamics (DDD) simulations. The main objective of DDD is to assist the theoretical description of material imperfections by filling the gap between the atomic scale and fully continuum models. The objective of our study is to investigate a possible inaccuracy in DDD simulations.

As a model problem, we consider two distinct dislocations of the opposite signs, gliding in their respective slip planes. Dislocation gliding is restricted to the channel of the persistent slip band (PSB), which serves as the convenient boundary. The interactions between the dislocation and PSB walls are simulated by elastic field of rigid dipoles which act as potential wells. The interaction stress field between two distinct dislocations is given by Devincre's formulas. As dislocations are pushed by the applied stress, they bow out and attract each other, either forming a dipole formation, or pass and escape each other. Our objective is to estimate the value of the applied stress needed for dislocations to pass. In our simulations, we employ the total stress and the total strain controlled regimes to obtain the upper and the lower estimate of the passing stress, respectively. The passing stress in the Browns interpretation [1] is identified with the fatigue endurance limit. The results of our numerical experiments indicate that the upper and lower estimate of the passing stress differ in less than 10%.

Dislocations are modeled as smooth closed or open planar curves evolving in time and their respective slip planes. Their motion is driven by the mean curvature flow

$$Bv = T\kappa + F, \tag{1}$$

where v denotes the normal velocity, κ is the mean curvature and F is the sum of all force terms acting on the dislocation curve in the normal direction. In this model B denotes the drag coefficient and T stands for the line tension.

The scalar motion law (1) is treated by means of the parametric approach resulting in the system of degenerate parabolic PDEs for the position of the dislocation [2, 3]. For the numerical simulations, we investigate semi-implicit flowing finite volume method [2, 3]. The numerical model is enhanced by the tangential redistribution which moves the discretization points along

the dislocation curve. Since the tangential terms do not affect the shape of the evolved curve, this technique enhances the numerical stability.

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References

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Ultrasonic characterization of beta-omega transitions in metastable beta-Ti alloys

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Elastic constants of both single crystals and polycrystalline aggregates of metastable β−titanium alloys with particles of both athermal and isothermal ω−phase were studied by ultrasonic methods. For the single crystals, it was observed that in the temperature range 0 °C – 80 °C the presence of these particles leads to stiffening and isotropization of the material and has also a significant impact onto the internal friction; much stronger effect onto the internal friction was observed for the athermal ω−phase particles than for the isothermal ones. The presence of the ω−particles leads also to stronger temperature dependence of the elastic constants. By comparison of elastic constants of samples with different volume fractions of isothermal ω−particles, the effective isotropic elastic constants of the ω−phase were calculated.
For the polycrystalline samples, the ultrasonic measurements enabled in-situ detection of formation and/or growth kinetics of the athermal ω-particles during thermal cycling.