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The Final Proceedings for Linking Processing to Performance Through Microstructure, 2 May 2004 - 5 May 2004

The objective of this workshop was to review recent European advances in the characterization of microstructure and the incorporation of microstructure into materials models that tie processing with mechanical properties. Topics of interest include microstructurally-informed constitutive modeling, microstructural evolution during processing, crystal plasticity approaches, representation of key aspects of microstructure within continuum finite element models, and probabilistic aspects of property prediction.

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Workshop Report: "Linking Processing to Performance Through Microstructure"

Breitnau (Freiburg), Germany

3 – 5 May 2004

Introduction:

The objective of this workshop was to review recent European advances in the characterization and representation of microstructure and how they can be used in linking processing and property models. Topics addressed included new approaches to three-dimensional quantification of material structure across all relevant length scales and the use of microstructural parameters in monotonic, cyclic and time dependent property models. Other topics of interest included probabilistic aspects of property prediction, microstructurally-informed constitutive modeling, crystal plasticity approaches and representation of key aspects of microstructure within continuum finite element models. The workshop was divided into five topical sessions over two and a half days.

Overview:

Session 1 was devoted to **Characterization of Microstructure for modeling.** Prof. Reiner Kircheim (University of Göttingen, Germany) described recent *ab initio* modeling of segregation to grain boundaries, considering the implications for grain boundary diffusion, grain growth and nucleation; he related the theoretical findings to published experimental measurements of grain boundary segregation. Dr. Mike Uchic (AFRL/MLLM, WPAFB, USA) described their work on three-dimensional microstructural profiling and micro-specimen machining/mechanical testing using *Focused Ion Beam Etching* in conjunction with SEM, Orientation Imaging and micro-compression testing. Prof. Colin Humphreys (University of Cambridge, UK) discussed the need for advanced electron microscopy for revealing micro- and nano-structures. He illustrated the need in relation to the development of Ga-In N light emitting alloys, where apparent atom clustering appears to be a consequence of microscope electron beam, rather than being an intrinsic part of the material structure. Prof. Hamish Fraser (The Ohio State

University, USA) described their work, complementary to AFRL/MLLM, in characterizing three-dimensional microstructures.

Session 2 was devoted to **Property Prediction.** Prof. Harry Bhadeshia (Univ. of Cambridge, UK) described his work on developing high strength steels by linking modeling from the atomistic to engineering property scales. His treatment of *Transformation Plasticity and Mixed Microstructures* gave a basis for designing mixed bainitic and austenitic steels for specific applications. Prof. Dierk Raabe (Max Planck Institute, Düsseldorf, Germany) reviewed a wide range of materials processes where interface characteristics were important. He asked the question of the level of knowledge of microstructure that was required for process modeling, observing that direct characterization of crystal rotations by orientation imaging can provide better validation than stress/strain measurements. Prof. Malcolm McLean (Imperial College, London, UK) described progress in making microstructure more explicit in modeling of superalloys: it is an output of advanced solidification models and an input of the Imperial College creep model, giving the potential of linking process and performance models. Prof. Tresa Pollock (University of Michigan, USA) discussed complementary work on modeling the yield stress of nickel-base superalloys from knowledge of the microstructure by coordinating and modifying previous knowledge. She also discussed work on rapid experimental characterization of the materials.

Session 3 was concerned with **Process Modeling.** Dr. Alain Jacot (Ecole Polytechnique Fédérale de Lausanne, Switzerland) linked a two-dimensional solidification model to a thermodynamic database to predict the microstructures in commercial aluminum alloys. The approach was used to simulate microstructures produced in commercial DC casting. Dr. Jeff Brooks (QinetiQ, UK) described their approach to the lifing of gas turbine components, encompassing fatigue and crack growth, and also their anisotropic creep model for single crystal turbine blades. Dr. Sammy Tin (Univ. of Cambridge, UK) discussed the modeling of thermo-mechanical processing through a state variable approach using constitutive equations linked to the evolution of grain- and micro-structure. He also described the linkage of models in the multi-stage forging of gas-turbine discs. Prof. John Humphreys (UMIST, UK) talked about deformation microstructures in aluminum and discussed how this influenced recrystallization. He confined the discussion to simple aluminum alloys indicating the roles of strain level and precipitate volume fraction on the recrystallization behavior.

Session 4 was devoted to **Dislocation Modeling.** Dr. Benoit Devincre (MEL, CNRS/ONERA, France) developed a model based on *discrete dislocation dynamics* to simulate strain hardening and dislocation patterning in structural materials. He pointed to the dangers of anomalous predictions associated with unrealistic periodic boundary conditions. The role of cross-slip is critical and consideration has been given to a range of proposed dislocation junctions. Dr. Holger Brehm (Fraunhofer Institute, Freiburg, Germany) developed a model of the creep of single crystal superalloys based on the evolution of dislocation density. This utilized a finite element realization of flow in the two-phase alloy. Dr. Daniel Weygand (University of Karlsruhe, Germany) presented a three-dimensional discrete dislocation dynamics model using limited glide systems and Lomer-Cottrell lock simulation. He showed that the stability of Lomer-Cottrell locks is sensitive to the loading path with implications cyclic loading. Dr. Dennis Dimiduk (AFRL/MLLM, WPAFB, USA) discussed the implication of their observations on micro-scale testing on early stage plasticity. The stress-strain curves show strong size dependence suggesting that the density of dislocation sources in the small diameter specimens may be too low to simulate the performance in bulk material. However, the tests constitute a powerful tool for investigating dislocation interactions as well as material heterogeneities.

Session 5 covered **Phase Field and FEM Modeling.** There were four presentations. Prof. Yunzhi Wang (The Ohio State Univ., USA) gave two talks. The first discussed simulating microstructure evolution using phase field modeling and covered work on both nickel-based superalloys and alpha/beta titanium alloys. The objective of using the phase field approach is to achieve quantitative prediction of microstructural features at experimentally relevant length and time scales. He demonstrated his results in prediction beta grain growth and grain boundary alpha thickening. Prof. Wang's second talk focused on simulation of dislocation behavior using phase field modeling. He centered his discussion on linking *ab initio*, atomistic and phase field modeling together for the case of nickel-based superalloys. Prof. Paul Van Houtte (Katholieke Universiteit Leuven, Belgium) described macroscale constitutive modeling for anisotropic plasticity. He started with a direct approach of mapping experimentally obtained microstructural texture information onto a two-dimensional finite element model. However, this approach doesn't lend itself easily to a three-dimensional FE mesh, so simplifications such as using geometrical grids with statistical distribution functions must be considered. Prof. Van Houtte also described how a crystal plasticity finite element modeling approach (CPFEM) leads to good grain interaction results, but gives disappointing results with a low number of elements, and takes too long to calculate. He further described other models, such as the advance Lamel model, and the advantages in terms of calculation speed, but limits in predicting strain gradients. Dr. Samuel Forest (Ecole de Mines, France) discussed his effort to connect single to polycrystal continuum plasticity through computational homogenization methods with consideration of size effects. He presented a comparison between finite element models, analytical models, and experiment from compact tension specimens. He intends to extend his future work to three-dimensional computations for polycrystal plasticity to include grain boundary effects such as damage and sliding.

Summary:

As with the previous workshop held in Breitnau last year, the meeting achieved its objective of identifying a strong European research activity in the field of microstructure-specific modeling. There is further scope for the development of US/Europe research collaborations in this area.