Interfacial Materials - Computational and Experimental Multi-Scale Studies

INCEMS: Grain growth modeling by a three-dimensional vertex dynamics simulation

L. Yue, D. Weygand, P. Gumbsch

The INCEMS project is funded by the EU within the Sixth Framework Program and coordinated by izbs. The objective is to study interfaces in perovskite ceramics by combining computational modeling with dedicated experimentation at all length scales with a strong, critical mutual validation. INCEMS started in August 2005 and will terminate in July 2009.

Coordinator:

- Prof. P. Gumbsch, izbs, Universität Karlsruhe, Germany

Partners:

- Prof. M. Hoffmann: Institut für Keramik im Maschinenbau, Universität Karlsruhe
- Prof. Adrian Sutton: Imperial College, London, UK
- Prof. Mike Finnis: Imperial College, London, UK
- Prof. Rudolf Podgornik: University of Ljubljana, Slovenia
- Prof. Martine Gautier-Soyer: Laboratory of Physics and Chemistry of Surfaces and Interfaces, CEA, Orsay, France
- Prof. Manfred Rühle: Max Planck Institute for Metals Research, Stuttgart
- Prof. David Cockayne: Department of Materials Science, University of Oxford, UK

The INCEMS project aims at demonstrating the computational predictability of complex properties of industrially relevant multifunctional perovskite ceramics, with nanometer-sized intergranular films by investigating and tailoring the interfaces.

Izbs contributes to the study of grain growth by means of a mesoscopic simulation approach, based on an improved three-dimensional vertex dynamics model for grain growth. This model is an interface tracking model, which explicitly follows the grain boundary structure evolution. The grain boundaries (GB) and triple lines are discretized and develop curved surfaces and lines. The simulation results are grain structures which were analyzed using statistical observables, such as grain size distribution functions and correlation functions between grain size and number of neighboring grains.

In Fig. 1 (a) and (b) a 2D cross section from experiment and from the 3D model are shown. The trace of the grain boundaries in both cross sections is curved. Several S-shaped cutting lines are found in both images.

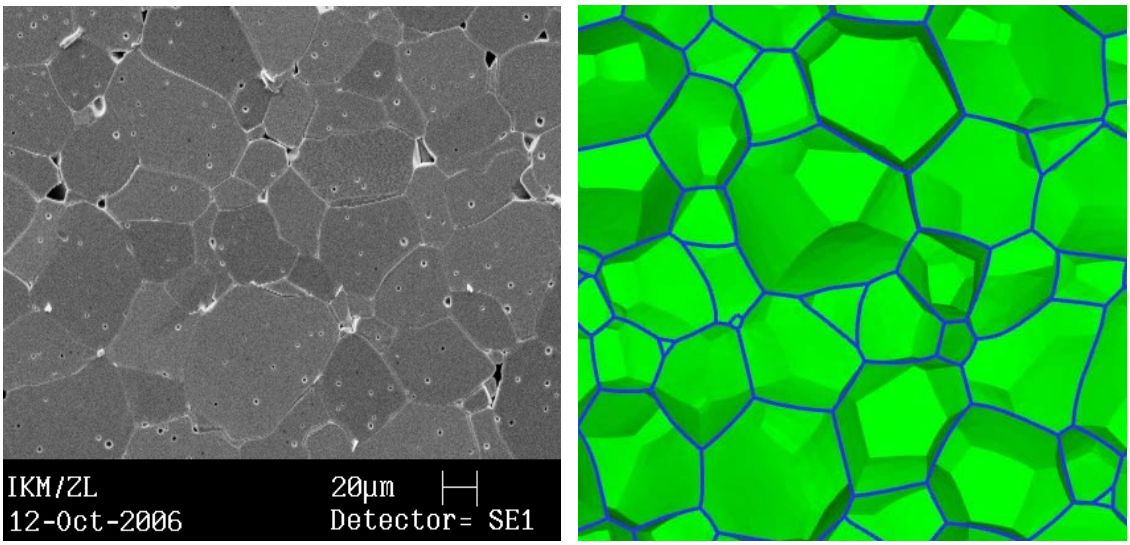

Fig. 1: 2D cross section from (a) experiment and (b) simulation

The present model allows the study of the influence of anisotropic GB properties. Recent research shows that the grain boundary property distributions are dependent on the grain boundary misorientations and boundary plane orientation. The fine discretion of grain boundaries allows for more precise anisotropic GB properties in simulation.

Abnormal Grain growth:
The occurrence of abnormal grain growth was observed for energetically and mobility favored GBs, as in the example in Fig. 2.

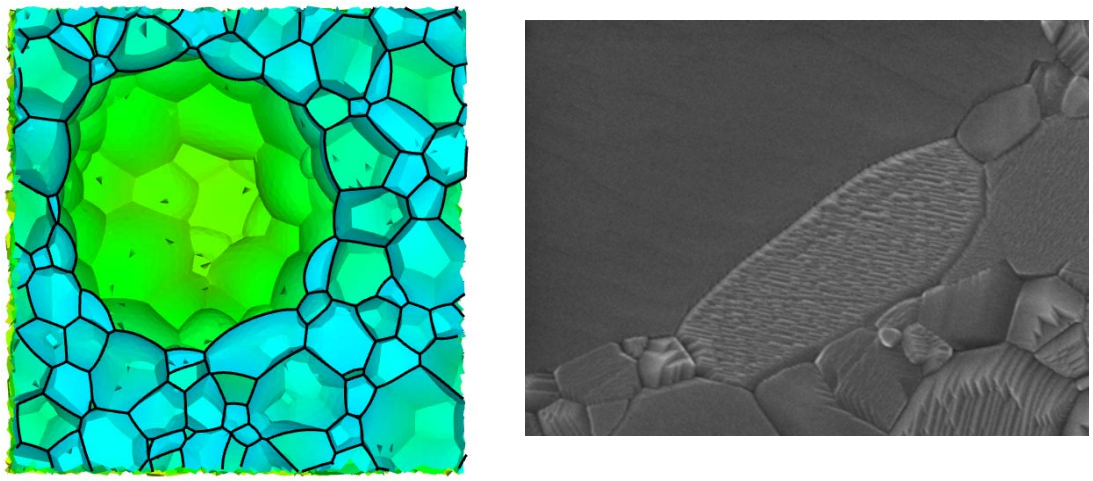

Fig. 2: Abnormal grain growth in simulation and experiments on STO Ceramics: (a) abnormal grain and matrix grains; (b) experiments performed at the IKM (M. Bäurer, M. Hoffmann)