ESRF	**Experiment title:** Linking grain growth anomaly in $SrTiO_3$ to the morphology of grains by diffraction contrast tomography	**Experiment number**: 23670 MA970
Beamline:	**Date of experiment**: from: 13.06.2010 to: 20.06.2010	**Date of report**: 06.10.2010
Shifts:	**Local contact(s)**: Loredana Erra	*Received at ESRF:*

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Report:

The aim of this experiment was to link the grain morphology of $SrTiO_3$ grains to the grain growth anomaly recently observed in this material [1]. We supposed changes in grain boundary faceting and thus grain boundary migration mechanisms as origin for the non-Arrhenius type of behaviour, resulting in drops in the effective mobility at two distinct temperatures, see figure 1. Hence we were interested in the fraction of globally flat boundaries and whether this number changes when going from one growth regime to another. Moreover, we wanted to compare the experimental data to simulation results from a mesoscale model [2] that used experimental data as input, in order to discriminate different grain boundary mobilities and energies used throughout the simulations.

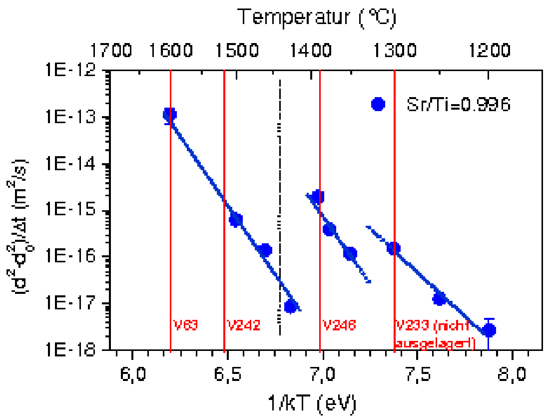

Figure 1: Samples that have been chosen for diffraction contrast tomography (marked as dots) and their effective mobility as a function of thermal activation energy.

Therefor, specimen representing the different growth regimes were picked, see figure 1, and measured before and after an ex-situ heat treatment that was expected to result in a coarsening of roughly 30%, see table 1. The reconstructed tomography datasets provide both shape and crystallographic orientation information and will thus give insight on changes in grain boundary faceting behavior. As far as we can see at this point, the data is in good shape and the first reconstructions yield promising results, see figure 2. A first before and after annealing comparison reveals a growth of approximately 15-20 %, corresponding crossections of the sample are shown in figure 3. Shrinking and growing grains can easily be identified, as can be the pore evolution, see figure 4. Once all the datasets are reconstructed, they will be analyzed in detail and used as input for mesoscale grain growth simulations.

Sample	Sintering	Annealing
V63	1h 1600°C	1h 1600°C
V233	6min 1600°C + 300h 1300°C	-
V242 A/B	2h 1420°C + 2h 1500°C	10h 1520°C
V246	2h 1420°C + 2h 1500°C + 10h 1390°C	10h 1390°C

Table 1: Details on the sintering and ex-situ annealing.

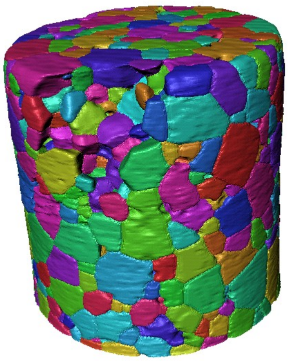

Figure 2: 3D reconstruction of V63 before annealing [3].

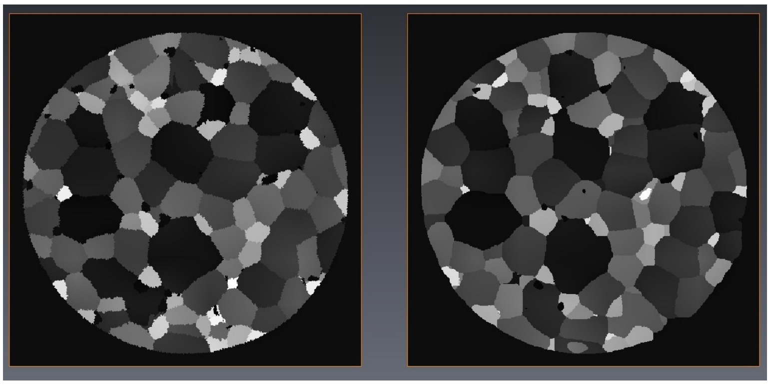

Figure 3: Cross section of V63 before and after anneling (1600 °C, 1 h).

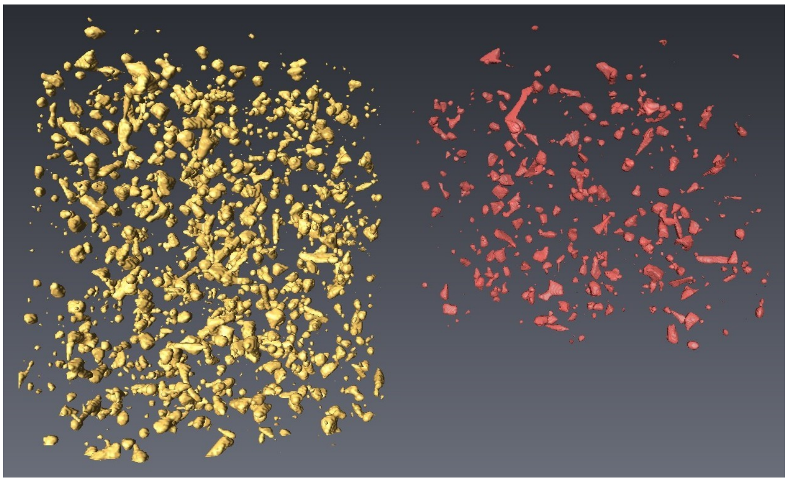

Figure 4: Pores in sample V63 before (left) and after (right) annealing.

Abstract of first publication [3]:

Experimental investigations in STO ceramics revealed a grain growth anomaly, that presumably originates in the interface anisotropy of these materials. However, the influence of anisotropic grain boundary properties on grain growth behaviour is to a large extend unknown. The present paper presents 3D grain growth simulations as a possible approach to understand the influence of anisotropic grain boundary properties on the collective behavior of the grain boundaries in a polycrystal during grain growth. Possibilities to compare 3D growth simulations with experimental 2D sections are discussed and a first reconstructed x-ray diffraction contrast tomography image of a $SrTiO_3$ specimen is presented.

[1] M. Bäurer, D. Weygand, P. Gumbsch, M. Hoffmann, Grain growth anomaly in strontium titanate, Scr. Mater. 61 (2009) 584–587.

[2] M. Syha, D. Weygand, A generalized vertex dynamics model for grain growth in three dimensions, Modeling and Simul. Mat. Sci. Eng., 18 (2010) 015010

[3] M. Syha, M. Bäurer, M.J. Hoffmann, E.M. Lauridsen, W. Ludwig, D. Weygand, P. Gumbsch, Comparing grain growth experiments and simulations in 3D, Proceedings of the 31st Risø Symposium 2010, accepted