Studies of texture, grain boundary character distribution, and relative grain boundary energies in Ca-doped Y_2O_3.

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Sept. 30, 2011
This report summarizes work carried out over the past four months

A. Texture Measurements:

Two 100 ppm Ca-doped Y_2O_3 samples were compared. The first was heated to 1700 °C and immediately cooled (referred to as NGG). The second was held at 1700 °C for six hours (referred to as AGG).

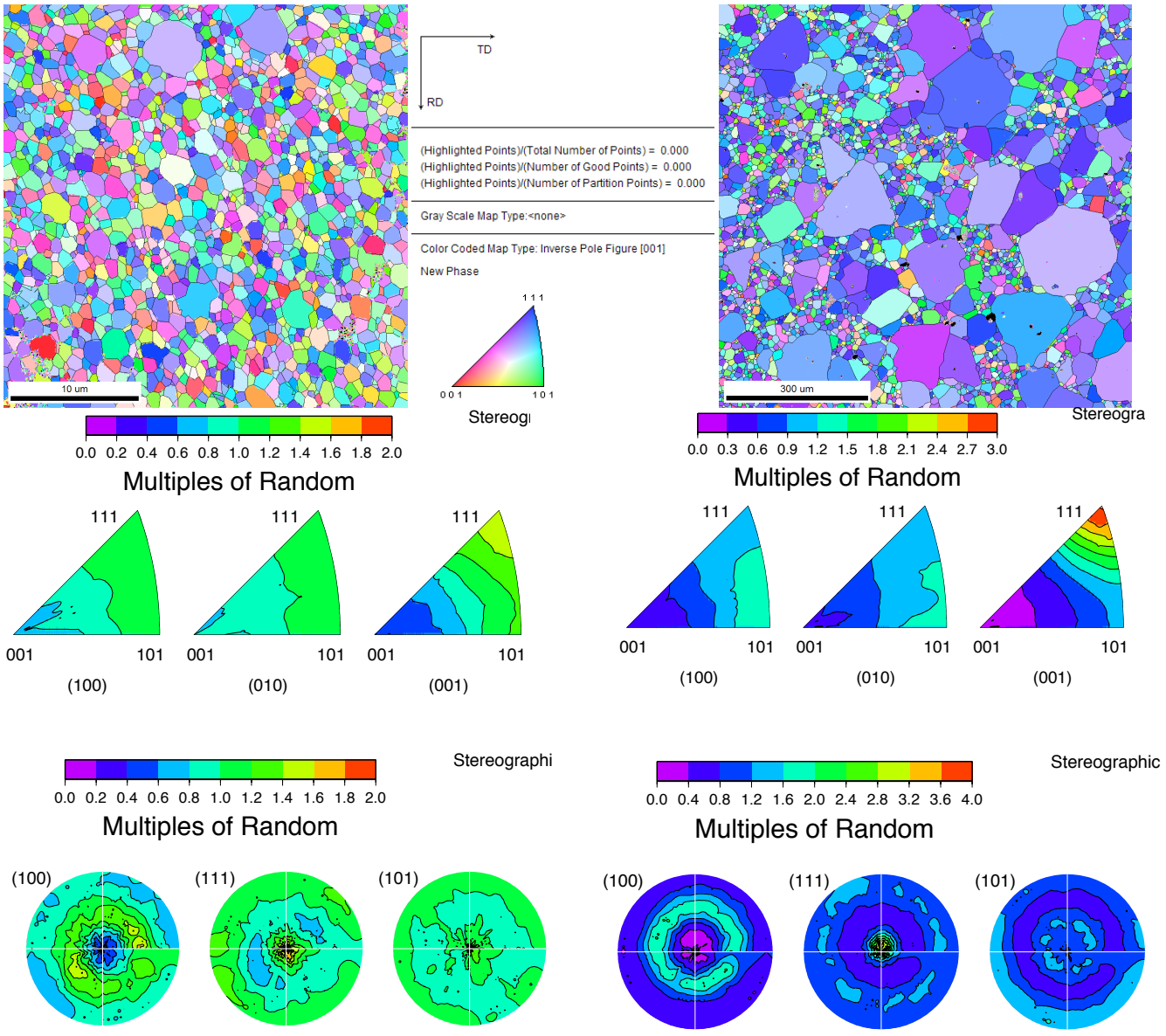

Figure 1: a) NGG inverse pole figure map of microstructure (10 μm scale bar) b) AGG inverse pole figure map (300 μm scale bar) c) NGG IPF d) AGG IPF e) NGG PF f) AGG PF

Inverse pole maps with superimposed reconstructed grain boundaries from each sample can be seen in Fig. 1 a and b. The grain orientation texture in each sample is quantified by the Inverse Pole Figures (IPF), in Fig. 1c and d, and Pole Figures (PF), Fig. 1e and f. The dominant color in the IPF map of the AGG sample is blue, indicating a dominant (111) orientation, while the NGG sample has a more random distribution. The IPF plots are consistent this observation, showing that the (111) [001] is strongly preferred with a peak around 3 MRD. The NGG sample does not have any peaks above about 1.5 MRD, and therefore has no significant preferred orientation. The data in the pole figures are consistent with the IPF maps.

2. Grain Boundary Plane Distributions (GBPD)

The GBPD of the NGG and AGG yttria samples can be seen in Fig. 2a and b respectively. From these distributions it is clear that there is a drastic difference in plane distributions between the samples. The NGG sample weakly favors {111} grain boundary planes, while the AGG sample strongly favors {001} planes. While the distribution is influence by the change in sample texture, the grain orientation texture change can not explain the difference in the GBPD.

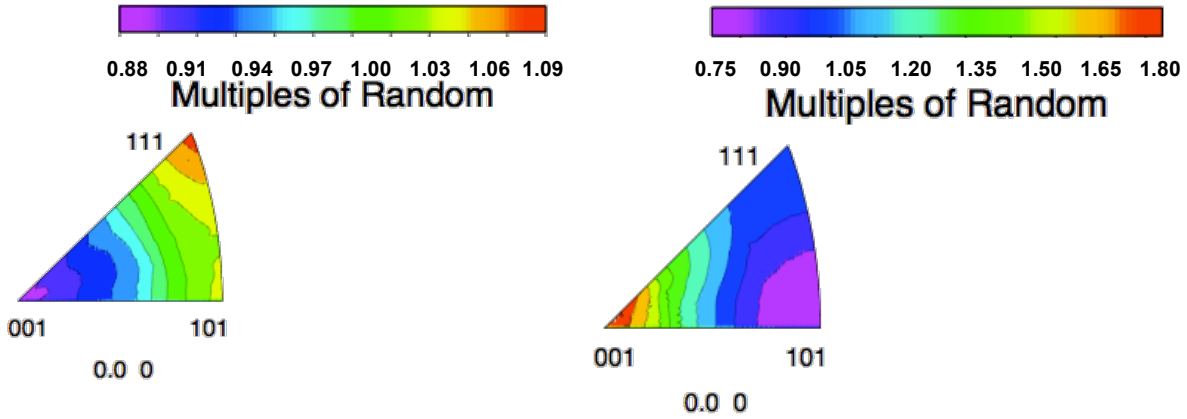

Figure 2: a) NGG GBPD b) AGG GBPD

3. Grain Boundary Character Distributions

Grain boundary plane distributions at fixed misorientations are shown in Fig. 3. The most notable peak in the distributions of both the NGG and AGG samples is the 45°/[100] at the (100) orientation. While the relative area of this plane boundary type is by far the greatest, it is relatively constant between the two samples. However, there are also differences. For example, the 60°/[111] NGG distribution shows MRD peaks surrounding but not at the (111) position while the AGG distribution shows a shift in the distribution with peaks at all of the {001} and {111} planes. The GBCD of pure yttria was studied previously by Dillon [J. Am. Ceram. Soc., **92** (2009) 1580-1585]. The GBPD reported in that study was most similar to the NGG sample of this study. However, when comparing the GBCDs of specific misorientations, there are a few significant differences between the two distributions. For example, the extreme peak at 45°/[100] found in this work is not present in the undoped yttria GBCD. This change in character could correspond the effect of the 100 ppm Ca doping.

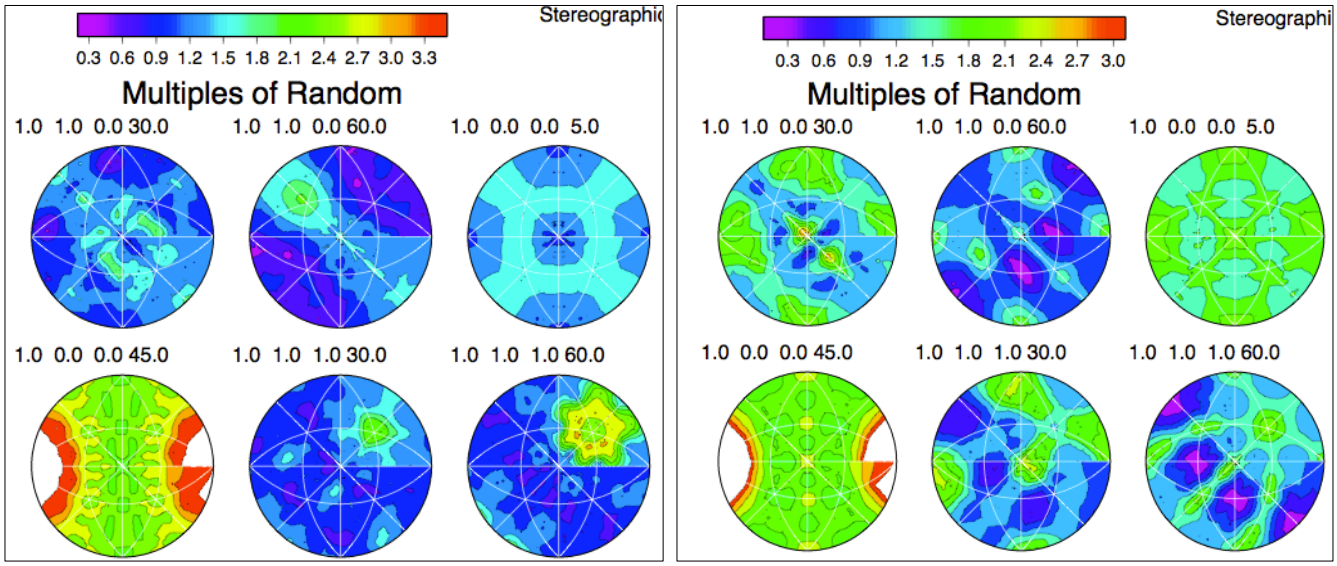

Figure 3. GBCD of NGG and AGG

4. Relative Grain Boundary Energies

The cumulative distribution function of the dihedral angles for the abnormal grain boundaries (AG-NG), normal grain boundaries in the AGG sample (NG-NG) and NGG grain boundaries (NGG) can be seen in Fig. 4. The average dihedral angle and relative energy for each distribution is also shown. From this information it is clear that there is a significant difference in the interfacial energies between the AGG sample and NGG samples. Furthermore, there is no difference between the boundaries surrounding abnormal and normal grains in the AGG sample.

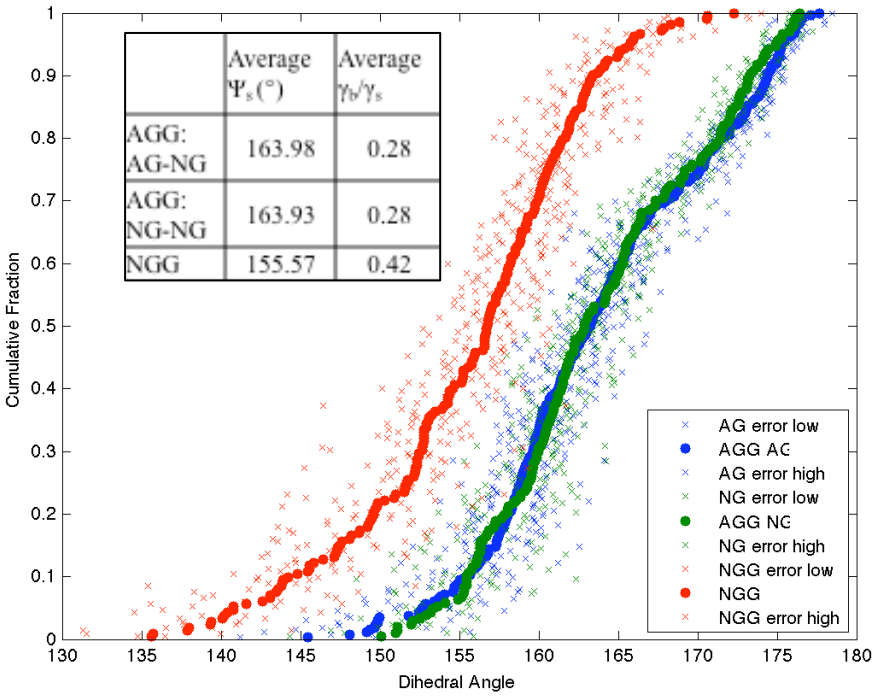

Figure 4. Cumulative distribution function comparing abnormal boundaries (blue), normal boundaries in AGG sample (green) and normal boundaries from NGG sample (red).

5. Findings

Ca doped yttria samples with the same composition, sintered at the same temperature but held for different times, have significantly different grain boundary character distributions and mean grain boundary energies. The presence of abnormal grain growth initiated a clear shift in the GBCD from a (111) preference in the NGG sample to (100) preference in the AGG sample. This indicates that the complexion transitions may occur on specific planes. Although the AFM results show there is no difference between the relative interfacial energies of the abnormal and normal grain boundaries in the AGG sample, the energies of boundaries in the AGG sample were lower than in the NGG sample. This work is consistent with the idea that the complexion transition, which caused the abnormal grain growth, changed the mesoscale grain boundary character and also affected the relative interfacial energies.

6. Future work

The main activities for the future are:

1. Draft a manuscript based on the above results and send to Harmer and Ma for input.
2. Begin work on Bi- and Sb-doped ZnO. The first step will be to fabricate samples.
3. We are also interested in conducting mesoscale studies on any other samples produced by groups in the MURI.