Geophysical Research Abstracts,
Vol. 11, EGU2009-10523, 2009
EGU General Assembly 2009

Neodymium -Yttrium interdiffusion in synthetic YAG bicrystals.

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The interdiffusion of Neodymium and Yttrium along a single grain boundary in synthetic Yttrium Aluminium Garnet (YAG) bicrystals is investigated. For the diffusion experiments Nd doped YAG thin-films are deposited on the bicrystal using Pulsed Laser Deposition, where the grain boundary is perpendicular to the thin film. Electron transparent foils are prepared using Focused Ion Beam (FIB) technique. Analytical and Energy-filtered High-Resolution Transmission Electron Microscopy (ATEM, HRTEM) shows that the YAG has crystalline structure along the grain boundary, amorphous material is absent. During the diffusion anneal, the initially amorphous thin-films crystallize. The crystallites grow epitactically on the bicrystal. Ultimately this leads to conversion of the thin film into an epitactic bicrystal, and the original grain boundary continues in the thin film.
Nd and Y concentrations were analyzed along the grain boundary using Energy Dispersive X-ray Spectroscopy (EDS) applying beam scans over an area of 40 nm by 20 nm per analysis.
To get better insight into the key physical processes, the system was modelled using a finite element method. Two different dynamic models were implemented. In a first, standard model the film is considered as a constant source for the volume and boundary diffusion in the substrate (Fisher's model). The alternative model was specifically designed to capture the actual experimental configuration. It accounts for the successive decrease of component diffusivity in the thin film, which is associated with its structural change from amorphous to crystalline during annealing. In this model the constant source approximation is dropped. The modelling results are compared to the experimental data. The comparison yields an estimate for the grain boundary diffusion coefficient.