MS16-P10

Determination of the crystal structures of an oxidized $TbDy_2Fe_6$ thin film by synchrotron radiation anomalous X-ray scattering

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The cubic Laves phase RFe_2 compounds (R= Tb and Dy) with cubic $MgCu_2$-type structure have giant room temperature magnetostriction constants. To make this compound as a thin film is very useful for the applications on Micro-Electro- Mechanical Systems However, as a thin film, it is apt to the oxidation of the thin film. To study the oxidation of RFe2 thin film is of interesting in the material science.

In this work, 160 nm $TbDy_2Fe_6$ thin films were prepared by magnetron sputtering and annealed in the range of temperature between 550 and 850 ºC. The structure of $TbDy_2Fe_6$ thin films were characterized by X-ray diffraction, and strong diffraction peaks of rare-earth oxides, Tb_2O_3 or Dy_2O_3 and other non-stoichiometric peaks were found. Since the lattice structure of Tb_2O_3 is very similar to that of Dy_2O_3, the composition of Tb_2O_3 and Dy_2O_3 cannot be determined by XRD separately. By using synchrotron radiation anomalous X-ray scattering, the amount of Tb and/or Dy oxidized at different annealing temperatures was determined. In addition, a pure Fe peak (110) was also detected using XRD. We use the anomalous X-ray diffraction and electron probe micro-analyzer to study this Fe diffraction peak.

With the anomalous X-ray scattering, the composition of the Tb_2O_3 or Dy_2O_3 was found to be the same as the sputtering target materials. It might be due to the same formation energies of oxides of Tb and Dy. In addition, 600 nm Fe clusters phase segregated from the bulk matrix without oxidation was also identified. These pure Fe cluster without oxidation might be due to the protection effect of Gd and Tb matrix.

In conclusion, oxidation of $TbDy_2Fe_6$ thin films were studied by X-ray anomalous scattering. The composition of Tb_2O_3 and Dy_2O_3 are similar to the composition of sputtering target. In addition, the Fe clusters phase segregated from the bulk matrix without oxidation was also identified.

Keywords: $TbDy_2Fe_6$, oxidation, anomalous X-ray scattering

MS16-P11

Structure- property relations and structural instabilities in high-temperature piezoelectric rare-earth calcium oxoborates RCa$_4$O(BO...

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Monoclinic (space group *Cm*) rare-earth calcium oxoborates (*RCOB*), RCa$_4$O(BO$_3$)$_3$ (R = rare earth element), have been studied for about 25 years because of their promising non-linear optical properties. These crystal species are isostructural with calcium fluoroborate, $Ca_5(BO_3)_3F$ [1], whose structure in turn is closely related to the one of hexagonal fluorapatite [2]. The substitution of tetrahedral PO_4 groups by planar BO_3 groups causes distortions which is the reason for the pronounced polar properties of the rare-earth oxoborates. Recently, the members of the *RCOB* family gathered interest as potential candidates for high-temperature piezoelectric sensing applications since they combine favorable properties like high melting point at around 1770 K, no reported structural phase transitions, high piezoelectric sensitivity and high electric resistivity [3]. Furthermore, the *RCOB* structure offers different possibilities for cation substitution which in principle allow for tuning of physical properties. Their low symmetry results in a high number of degrees of freedom regarding the anisotropy of physical properties.

We studied heat capacity, thermal expansion as well as dielectric, piezoelectric and elastic properties of $GdCa_4O(BO_3)_3$ between 100 K and 1473 K using differential scanning calorimetry, dilatometry and resonant ultrasound spectroscopy. Contrary to the reported lack of phase transitions, all investigated physical properties undergo reproducible discontinuities at around 1000 K. X-ray diffraction experiments on quenched samples indicate a gradual increase of cation disorder starting roughly at around 1000 K. Therefore, a glass-like transition from static to dynamical cation disorder is likely responsible for the observed discontinuities. First results indicate only a minor influence of the glass-like transition on the electromechanical properties.

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