at the Fe/MgO(100) interface do not detect any oxygen diffusion in the Fe film showing a sharp interface with the Fe crystallographic cell tetragonally distorted to match the MgO crystal lattice. These results will be discussed in relation to the magnetic properties of the systems.
[1] P. Luches et al, Phys. Rev. Lett. 96, 106106 (2006).

Keywords: interfaces, X-ray absorption fine structure, thin films

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Surface X-ray diffraction studies of CaF_2(110)/Si(001) interface formation

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In the earlier studies [1, 2] it was found that an interface of CaF_2(110)/Si(001) with non-trivial relations was formed during CaF_2 epitaxial growth on Si(001) surface at high temperature. The atomic structure of this interface was related to the formation of the wetting layer consisting of nanostripes running along [110] direction. In order to investigate the structure of the interface *in situ* surface X-ray diffraction (SXRD) measurements were carried out at the BL13XU of SPring-8. CaF_2 of 0.7-2.0 monolayer was grown on Si(001) substrate and over 40 in-plane reflections and 8 fractional order rods were measured. SXRD revealed the 3×1-like surface reconstruction (fig. 1) which is consistent with the electron diffraction studies [2]. A two-dimensional structural model was constructed based on the electron density distribution obtained from in-plane reflectioin data. The intensity profiles along the rods, reflecting the electron density distribution across the interface, suggested that more than one molecular layer were involved in the formation of the interface wetting layer.

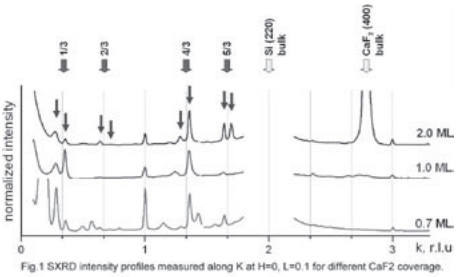

Fig.1 SXRD intensity profiles measured along K at H=0, L=0.1 for different CaF2 coverage.

[1] T. Sumiya et al., Surf. Sci. 376, 192 (1996).
[2] L. Pasquali et al., Phys. Rev. B72, 045448 (2005).

Keywords: surfaces and interfaces, surface diffraction, *in-situ* experiments

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Electroic states at the interface of Fe/MgO magnetic tunneling junction

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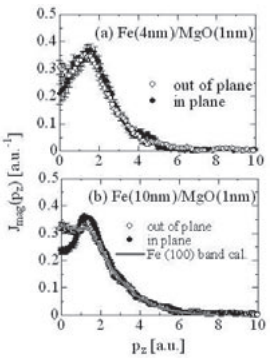
Recently fully epitaxial Fe/MgO/Fe MTJs have the likelihood of an extremely high MR ratio because of the coherent tunneling effect. For conservation of wave function coherency, an electronic structure at the interface is important. In this paper we discuss the electronic states at the interface of Fe/MgO magnetic tunneling junction by measuring magnetic Compton profiles (MCPs). Fe(xnm)/MgO(1nm) (x=4,10) multilayes were fabricated on Si(111) substrates and Al foil substrates by R.F. sputtering. Total thickness was adjusted to about 1000nm. The texture of Fe(200) and MgO(200) was confirmed by XRD measurements. No Fe oxide diffraction peak was observed. Magnetization measurements showed magnetic dead layer of 1nm at the interface. The MCP measurements were carried out at SPring-8-BL08W and KEK-PF-ARNE1A1. Fig.1(a),(b) show the MCPs of the Fe/MgO multilayers. The “hollow” around the pz=0 is deeper in the case of the Fe(4nm)/MgO(1nm) than Fe(10nm)/MgO(1nm). This indicates existence of relatively large spin polarization of conduction electron at the interface and suggests that the spin polarization of conduction electron remain although the Fe3d magnetization disappears.



Keywords: Compton profiles, multilayer films, interface characterization

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Thin film structures of epitaxial chromium on MgO(001) substrates by MBE

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Thin films of chromium (Cr) were epitaxially grown on MgO(001) substrates by means of molecular beam epitaxy (MBE) and studied by in-situ reflection high energy electron diffraction (RHEED) and ex-situ X-ray diffraction. Depositions of the Cr films were carried out from room temperature to 973K with vacuum of the order of 10-5 Pa. Epitaxial relations of Cr(001)//MgO(001) and Cr[100]//MgO[110] were obtained. We find that Cr(001) layers grown at the temperature higher than 673K and slow deposition rate of 0.1 nm/s shows 2X2 surface reconstructions. Epitaxial growth progressed further, clear horizontally-elongated RHEED streaks were found when the azimuth of the incident electron beam was parallel to the Cr[100] and superposed to usual streak and spotty pattern. Horizontal streaks were observed under following conditions; (1) low deposition rate and (2) high substrate temperature. Horizontal RHEED streaks can be speculated that the Cr thin films have wire-like structures along with [110] direction of Cr layer and was somewhat related to the existence of oxygen in the residual gas. X-ray diffraction from the Cr film, however, revealed that no evidence of chromium oxide, such as Cr_2O_3, was found.

Keywords: thin-film epitaxy, RHEED, MBE

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Thermally induced structural transformation in Co films for giant magnetoresistance spin valves

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The contribution is devoted to correlation between structural and magnetic properties of cobalt thin films exposed to vacuum annealing which are applied in giant magnetoresistance spin valves with current induced magnetization switching developed in our laboratory. The films of 40-130 nm thicknesses were deposited by electron beam evaporation onto Si wafers and treated by rapid thermal annealing up to 600℃. Thickness, surface/interface roughness and density profile of the films were determined by X-ray reflectivity. X-ray diffraction was measured in symmetrical reflection and grazing incidence geometries. As-prepared films exhibit modified near-surface region and roughness of 1 nm which was more than doubled on 600℃/1hour annealing. The film thickness decreased by 2-3% and the density increased accordingly. These changes are presumably connected with structural transformation observed in the films which was studied in detail on the 40 nm thick sample. The starting structure showed one broad diffraction peak around 44.5 degrees with a shoulder on the low-angle side which could be fitted as overlap of 100 and 002 diffractions of hexagonal close-packed (hcp) Co phase with the grain size of 14 nm. A similar analysis on a series of annealed samples revealed a transformation into (111) textured face-centered cubic (fcc) phase starting at 300℃ which was completed on 600℃ /1hour annealing with the grain size of 30 nm. This phase remained stable at room temperature. Longitudinal magneto-optical Kerr effect measurements showed enhancement of coercivity by a factor of two and loss of its azimuthal dependence which is in line with more degrees of freedom for spin reorientation in fcc structure. In thicker Co films, hcp and fcc phases coexist already in the as-deposited state.

Keywords: magnetic film, rapid thermal processing, structural transformations

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Gas deposition growth of ytterbium nanoparticles

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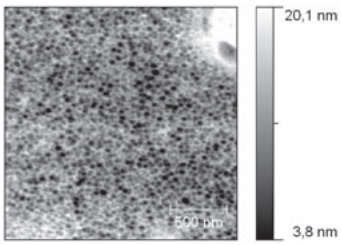
Formation of lanthanides' nanoparticles has become significant in basic research as well as some application to nanotechnology. Ytterbium is one of the most interesting elements in lanthanide because of its unique physical and chemical properties. In the present study, the gas deposition method has been employed to prepare the particles with wide variety of sizes. Metallic ytterbium has been evaporated by heating (300~650ºC, melting point is 824ºC) in He environment (0.5~11 Pa). The particles are formed by solidification and aggregation during the collisions with He gas molecules. A glass substrate, of which backside is water-cooled, is put at close position (~10mm) from the top of the K-cell, to collect floating particles. Figure 1 shows a typical AFM image of the ytterbium particles (0.49 Pa, 400ºC, 1 hour deposition). The shape of particles is almost spherical with relatively narrow size distribution. Patricles are randomly spread on the substrate without any preferred organization. Grazing incidence X-ray techniques were used to determine the structures. In the present study, the use of N_2 gas has been also attempted. The comparison will be discussed in the presentation.



Keywords: nanoparticles, X-ray characterization, AFM

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Highly spin-polarized interfaces between a half-metallic Heusler alloy and silicon

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Finding out ferromagnet/semiconductor interfaces which show high spin polarization at the Fermi energy is one of the key issues for achieving efficient spin injection into semiconductor. First-principles calculations have so far proposed many ferromagnets completely spin-polarized at the Fermi energy (half metals). However, it is also pointed out from theory that those half metals rarely keep the high spin polarization at interface. Regarding half-metal/Si heterostructures, for example, no highly spin-polarized interface has been predicted, though spin injection into Si is of great importance for developing silicon-based spintronics devices. In this work, we have investigated the electronic and structural properties chiefly of Co2FeSi/Si and CoFeSi/Si interfaces using first-principles density-functional calculations. The half-metallic properties possessed by both Co2FeSi and CoFeSi in the bulk state are found to be almost preserved at specific (110) interfaces. Besides, these highly spin-polarized interfaces turn out to have the lowest energy of the (110) interfacial patterns studied here. The nearly half-metallic character at the interfaces is also found in the densities of states projected onto delocalized sp-orbitals; this fact suggests that the high spin polarization is closely related to transport properties and, accordingly, to spin injection into Si. Possibility of similar interfacial half-metallicity will be further discussed for other heterostructures consisting of a Heusler alloy and a group IV semiconductor.

Keywords: half metal, spintronics, *ab-initio* calculations

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In-situ XRD study of thickness dependence of crystallization of amorphous titanium dioxide films

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