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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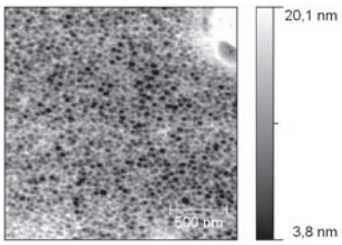
Formation of lanthanides' nanoparticles has become significant in basic research as well as some application to nanotechnology. Ytterbium is one of the most interesting elements in lanthanide because of its unique physical and chemical properties. In the present study, the gas deposition method has been 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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The excellent properties of titanium dioxide films (e.g. photocatalytic activity, hydrophilicity) largely depend on their phase composition, crystallinity and microstructure. Crystallization of amorphous films with different thickness (50-2000 nm) was investigated by in-situ isochronal and isothermal annealing at different temperatures and compared with the post-annealing of both amorphous and nanocrystalline films. The X'Pert Pro with MRI high-temperature chamber in parallel beam was used. The time dependences of crystallization were studied at low temperatures (180, 220℃). They could be well described by modified Avrami equation applied to the intensities of diffraction peaks $I = 1\text{-}\exp[-b(t-t_0)^n)]$. The exponent n was in the range 2-2.5 and slightly increasing with the film thickness. The initial time t_0 of crystallization (non-zero intensity) increases nearly exponentially with the decreasing thickness while the slope b increases significantly for thicker films. Typical time necessary for the crystallization of the whole film volume at the above temperature varied from several hours for thicker layers to about ten days for the thinnest films. Fast crystallization of the order of minutes appeared at 230 ℃ for thicker films and went up to 290℃ for the thin film (below 100 nm). Weak texture was changing during the crystallization. Significant shifts of diffraction peaks with the temperature were observed and tensile residual stresses were confirmed by the $\sin^2\psi$ method for different diffraction peaks. They decrease with the increasing film thickness. Line profile analysis shown the growth of relatively large crystallites (100 nm) already at the beginning of crystallization. Reflectivity indicates increase of surface roughness with the thickness.

Keywords: titanium oxide compounds, thin films and multilayers, crystallization

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Compositional analysis of $LaMnO_3$-$LaCoO_3$-$LaNiO_3$ thin-film thermoelectric property diagrams

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High-throughput combinatorial mapping is a state-of-the art screening technique for accelerating the selection and introduction of thermoelectric materials into the manufacturing process. A $LaMnO_3$-$LaCoO_3$-$LaNiO_3$ single-crystalline continuous spread combinatorial thin film library has been deposited onto a 50.8 mm diameter $LaAlO_3$ (100) substrate using home-grown targets via pulsed laser deposition (PLD). PLD occurred inside a vacuum chamber with a partial O_2 pressure of 13.3 Pa and at a heater temperature of 600 °C. Short duration KrF excimer laser beam pulses (25 ns) were used to strike the targets generating a plume of the vaporized materials which deposited onto the substrate. Inspired by our development of a high-throughput screening tool used to map out thermoelectric (TE) property variations as a function of wafer position, along with their technological importance, the cubic (*Pm*-3*m*) perovskite La*M*O_3 (*M* = Mn, Co, Ni) materials have been selected to generate a ternary library, which has been analyzed by X-ray diffraction (XRD) using a General Area Detection Diffraction System with a grid matrix, and compositional mapping wavelength-dispersive spectrometry (WDS). The phase diagram from the combination of the structural phase XRD data and compositional mapping WDS data, allows for a correlation with the TE properties (Seebeck coefficient, electrical conductivity, and power factor) obtained from the screening tool as a function of composition. The technique demonstrated here is expected to rapidly advance the exploration of thermoelectric perovskite oxides in comparison to conventional trial-and-error methods.

Keywords: thermoelectric materials, combinatorial library design, perovskite oxides

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Crystal structure and valence distribution of artificial superlattices $[(LaMnO_3)_m(SrMnO_3)_m]_n$

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The crystal structure and the valence distribution of Mn ions have been studied in the artificial superlattices, $[(LaMnO_3)_m(SrMnO_3)_m]_n$, utilizing X-ray scattering techniques. The high quality superlattices were fabricated, and all the films indicate an insulating behavior without reference to the periodicity *m*.The crystal structure of the films was determined by the structural analysis. The obtained stacking structure of $[(LaMnO_3)_m(SrMnO_3)_m]_n$ is consistent with the designed structure. The periodicity slightly deviates from the designed value and *m* becomes non-integer value. The Mn valence distribution was evaluated in the films by the resonant X-ray scattering technique. In these artificial superlattices, as a result, the Mn valence state is dominated by the La/Sr layers and is the rectangular wave from 3+ to 4+: The charge modulation spreading over a few layers near the interface could not be observed. $[(LaMnO_3)_m(SrMnO_3)_m]_n$ film with the rectangular wave of Mn valence state was elucidated to be intrinsically insulative.

Keywords: resonant X-ray scattering, charge ordering, superlattice structure

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Growth control of perovskite-related oxide thin films

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Perovskite-related oxides are materials showing interesting features. In order to realize functional devices taking advantage of these materials, top quality thin films for different applications are always necessary. However, it is not easy to grow such films and many criteria have to be fulfilled. The degree of complexity enhances significantly for muticomponent materials such as high-Tc superconductors, giant magnetoresistive materials, heterostructures,