

Abstracts for poster presentations
No. 01 - 09

No. 01

First-principles prediction of the control of magnetic properties in Fe-doped GaSb and InSb

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Recently, Fe-doped semiconductors have been attracting much attention as ferromagnetic semiconductors due to the possibility that they may exhibit high Curie temperatures and low power consumption and that they may be useful for high-speed spin devices. High Curie temperature ferromagnetism has been observed in Fe-doped InAs, from which both *n*- and *p*-type ferromagnetic semiconductors can be fabricated. In order to obtain a higher Curie temperature than that of (In,Fe)As, we have focused on GaSb and InSb as host semiconductors. Actually, Curie temperature higher than the room temperature and *n*-type dilute magnetic semiconductors (DMSs) were experimentally observed. For example, the Curie temperature of the Fe 25% doped GaSb is about 350 K. The Fe 16% doped InSb becomes *n*-type DMS and shows the Curie temperature of 330 K. Although the inhomogeneous Fe-rich regions are formed in both systems, the Fe atoms keep the zincblende structure of the host semiconductors without any ferromagnetic secondary precipitation such as FeSb [1,2].

We have investigated the electronic structures, magnetic properties, and structural stability of Fe-doped GaSb and InSb by using the Korringa-Kohn-Rostoker Green's function method within density functional theory. We have found that the isoelectronic Fe-doped GaSb and InSb have strong antiferromagnetic interactions due to the super-exchange mechanism. By considering artificial changes in the Fermi level, we have found that the magnetic exchange coupling constants in these systems exhibit universal behavior. Antiferromagnetic-ferromagnetic transitions occur for both *n*- and *p*-type doping, and this behavior can be well understood in terms of the Alexander-Anderson-Moriya mechanism. The Fermi level dependence of the chemical pair interactions also shows characteristic features, which can be reasonably explained by magnetic frustration and the nature of the covalent bond. Our multi-scale simulations show that finite Curie temperatures are realized in *n*- and *p*-type regions. For *p*-type doping, the spinodal nano-decomposition caused by annealing drastically enhances Curie temperature. However, for *n*-type doping, the initial phases have higher Curie temperatures than the final phases. Based on the results of our calculations, we propose

that high Curie temperatures may be realized and that the magnetic states of (Ga,Fe)Sb and (In,Fe)Sb may be manipulated by controlling the gate voltage, chemical doping, and annealing process. Such features will be very important for next-generation semiconductor spintronics [3].

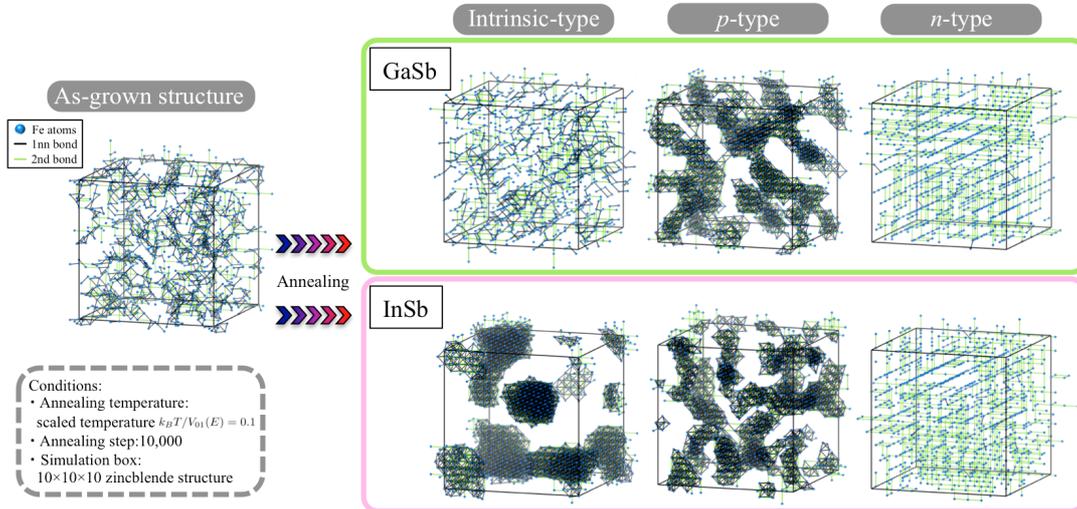


Fig. 1. Snapshots of the Monte Carlo simulation for the spinodal nanodecomposition in (Ga,Fe)Sb and (In,Fe)Sb. Initial phase and annealed phases of intrinsic-, p -, and n -type (Ga,Fe)Sb and (In,Fe)Sb after 10,000 Monte Carlo steps.

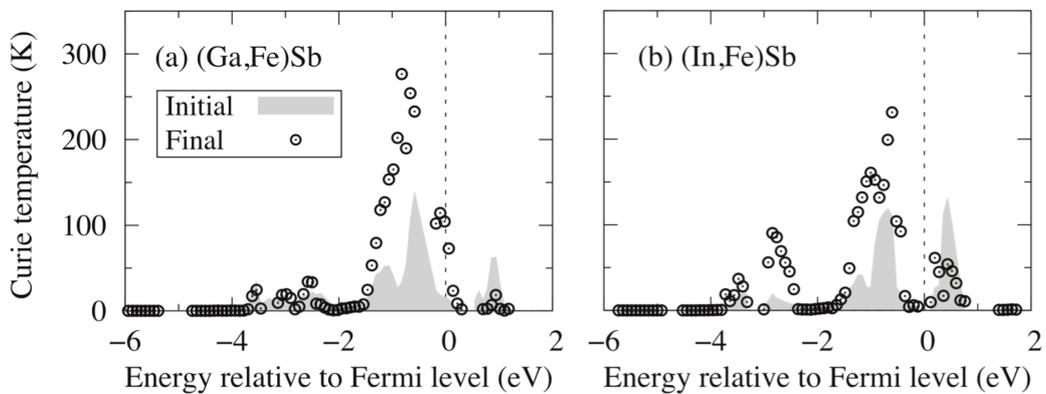


Fig. 2. Curie temperature of (a) (Ga,Fe)Sb and (b) (In,Fe)Sb for the initial (gray areas) and final (points) phases calculated with the random phase approximation as a function of the Fermi level shift. The Fe concentration is fixed at 20%.

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No. 02

**Size effect on the mechanical behavior of
single crystalline Fe-31.2Pd (at%) micropillars**

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The size effect on the mechanical behaviors of single crystalline Fe-31.2Pd (at%) micropillars with four different pillar diameters (approximately 2 μm , 1 μm , 500 nm and 400 nm) were studied by compressing in the [001] direction. Both the Young's modulus and yield stress increase with the decrease of pillar diameter. The main defects in the plastically deformed pillars are the {111} deformation twins, which could be covered by high density of dislocations after further plastic deformation in a 400 nm pillar. A repeatable elastic-like strain $\sim 4\%$ was observed for more than 40,000 cycles.

No. 03

Design of super-high- T_C high-entropy ferromagnetic semiconductors in Fe-doped III-V compound by spinodal nano-decomposition and volume compensated codoping

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Design and realization of super-high-Curie temperature (T_C) magnetic semiconductors, in which the exchange interactions can be controlled by gating, are essential for the realistic application of semiconductor nano-spintronics.

Recently, Fe-doped III-V-based narrow-gap diluted magnetic semiconductors with high- T_C are successfully grown by MBE, and T_C goes up to above room temperatures [1]. Based on the three general design rules of (1) the volume compensations [VC] by codoping with the substitutional (S) Fe impurity [Fe(S)] and the interstitial (I = tetrahedral (*tetra.*) or octahedral (*octa.*) interstitial site) Fe impurity [Fe(I)] [2], (2) spinodal nano-decomposition [SND] of Fe(S) and Fe(I) caused by the low solubility [3], and (3) high-entropy ferromagnetic semiconductors [HEFS] with reducing the Gibbs's free energy ($F = E - TS$) by increasing the entropy (S) in the disordered and high-concentrations of Fe(S) and Fe(I) with codoping [4], we design the super-high- T_C ($T_C > 1000\text{K}$) HEFS in Fe-doped III-V compound by computational nano-materials design [5]. Fe(S) at the III-element site reduces the volume, while the Fe(I) (I = *tetra.* or *octa.* interstitial site) expands the volume in III-V compounds, such as GaAs, GaSb, InAs and InSb, which is called volume compensation. The solubility of Fe(S) and Fe(I) are low due to the positive formation energy, so that the SND occurs due to the positive mixing energy. Based on the codoping of isoelectric Fe(S) and triple donors of Fe(I) with high concentrations more than 15~25% in the thermal non-equilibrium crystal-growth condition, we design the HEFS caused by high-doping concentrations with super-high- T_C based on the strong ferromagnetic double exchange interactions between the Fe(S) and Fe(I) caused by SND.

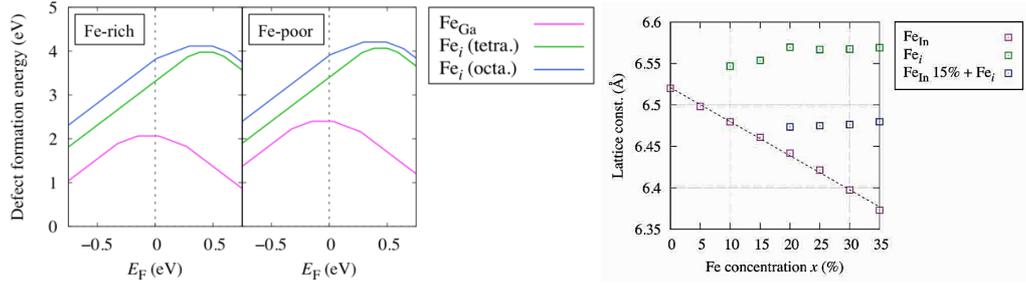


Fig.1: Defect formation energy of Fe at Ga-site (Fe_{Ga}), tetrahedral (Fe_i (tetra.)) and octahedral (Fe_i (octa.)) interstitial sites in GaSb in the Fe-rich and Fe-poor crystal-growth conditions (see the left two figures). Lattice constants vs. Fe concentration at the In-site (lower squares in the right figure) and at the interstitial site in InSb (upper squares in the right figure). After the doping of Fe 15% at the In-sites, then Fe 15% doping at the octahedral interstitial sites, the successive doping indicates V-shape dependence in the lattice constant due to the volume compensations (see the middle in the right figure).

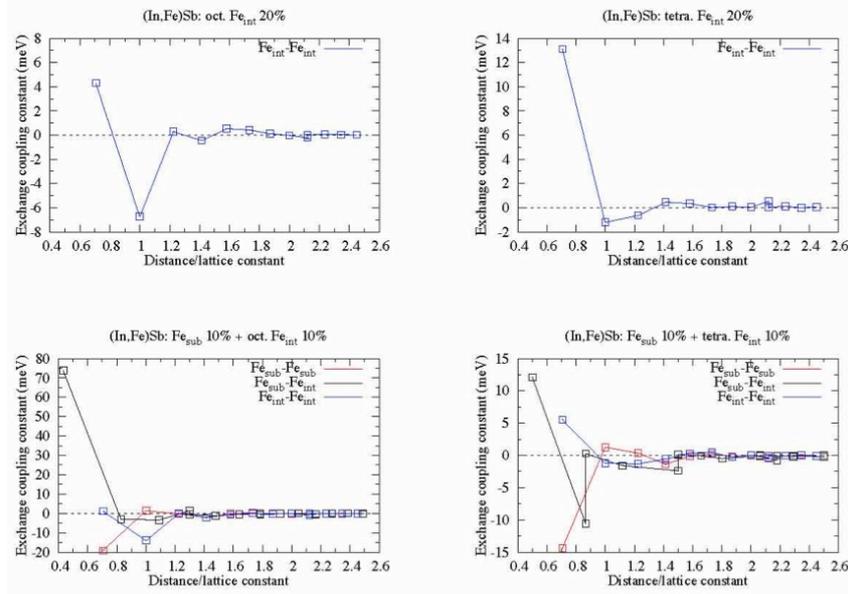


Fig. 2: Exchange interaction vs. distance between Fe impurities at the substitutional (sub.) and interstitial sites (int.) in InSb. It indicates the anti-ferromagnetic super-exchange interaction between the substitutional Fe, on the other hand, the ferromagnetic double exchange interaction becomes dominant between the substitutional and interstitial Fe impurities, and also between the interstitial impurities, where the carriers are caused by the triple donors of interstitial Fe_{int} .

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Fano effect in the transport of an artificial molecule

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The Fano effect [1] is a ubiquitous phenomenon arising from the interference between a discrete energy state and an energy continuum. It appears in various physical phenomena, for instance, in atomic photoionization, neutron resonance scattering, photoemission, and so on. In mesoscopic systems, too, the Fano effect was demonstrated in a quantum dot embedded in an Aharonov-Bohm ring, where asymmetric Coulomb peaks (“Fano lineshapes”) emerge instead of conventional Coulomb peaks with Lorentzian shape [2]. As the Fano effect in nanostructures is attracting many researchers [3], it is of significance to explore electron transport based on this effect in various systems to deepen our understanding of mesoscopic transport.

We experimentally address this effect in an artificial molecule [4], so-called double QDs (DQD), which is two lateral QDs fabricated on conventional GaAs/AlGaAs two-dimensional electron gas system (2DEG) and coupled in series. Conductance measurements for DQD are performed by the standard lock-in technique in a mixing chamber in a dilution refrigerator with a base temperature below 30 mK at zero magnetic field. We found that, when the coupling strength between the leads and QDs is small, the charge stability diagram of the system shows a well-known honeycomb lattice structure that is characteristic of a DQD system. On the other hand, as the coupling increases, a honeycomb structure consisting of the Fano lineshapes is observed to emerge. Our experiment is the first to realize the Fano effect in the artificial molecule.

We assume that the origin of the energy continuum that is necessary for this effect to occur is a strongly-coupled state between the two leads across DQD. Since such a state has large energy width, it eventually works as energy continuum. It coexists with the two discrete energy states in DQD, which have narrower energy width, resulting in the Fano effect. We confirm this scenario by numerical simulation based on the T-matrix method, which can satisfactorily reproduce our observation. Our achievement [4] constitutes a clear example demonstrating the ubiquitous nature of the Fano effect in mesoscopic transport.

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Magnetoresistance and Hall resistance measurements in triangular antiferromagnet Ag_2CrO_2 thin film

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Since the discovery of graphene in 2004, there have been many reports on two-dimensional (2D) materials. Especially, 2D materials showing some phase transitions have attracted much attention in terms of the Mermin–Wagner theorem. Recently, two independent groups reported 2D ferromagnetic materials [1,2], which could be useful for future atomic-layer spintronic devices. The motivation of the present study is to find some conductive 2D antiferromagnets and fabricate spintronic devices with them.

Ag_2CrO_2 is one of the layered triangular antiferromagnets with an electrical conductivity [3]. This material shows an antiferromagnetic transition at $T_N = 24$ K and exhibits a complex magnetic state, the so-called *partially disordered (PD) state*, below T_N [4]. When magnetic moments are arranged on a triangular lattice, it is well-known that the magnetic moments have a large frustration because of the geometrical effect. In this situation, it is theoretically predicted that a unique thermodynamic state, i.e., PD state, appears at finite temperatures [5]. However, the magnetic structure of the PD state is still unclear because the single crystal has not been prepared yet.

In this work, we have developed a new method to obtain higher quality thin films of Ag_2CrO_2 from the polycrystalline samples as shown in Fig. 1, and performed magnetotransport measurements. Figure 2 shows a typical magnetoresistance near the T_N . We observed a clear spin-flip process in the thin film samples, which has never observed in the polycrystalline ones. In the presentation, we will also discuss some results of Hall measurements.

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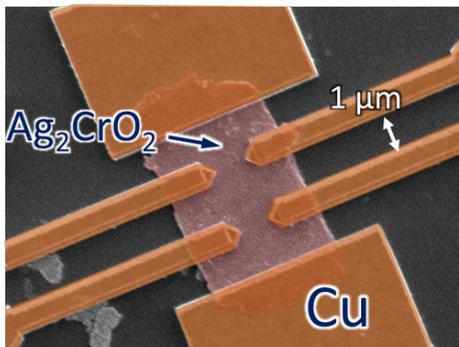


Fig.1 : Scanning electron microscope image of an Ag_2CrO_2 device.

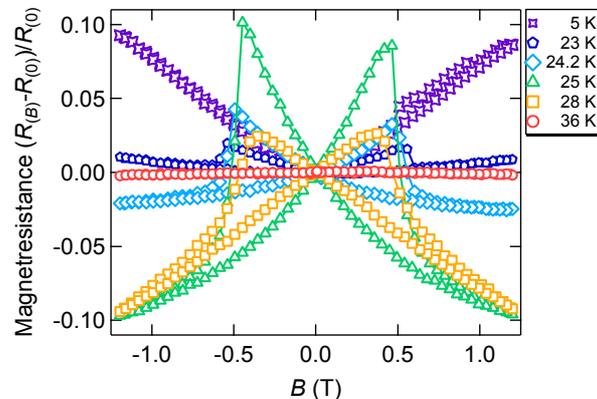


Fig.2 : Magnetoresistance of the Ag_2CrO_2 thin film at different temperatures. The magnetic field is applied perpendicular to the plane.

**Large anisotropic magnetoresistance induced by a proximity effect
in an InAs / (Ga,Fe)Sb quantum well heterostructure**

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Fe doped narrow-gap III-V ferromagnetic semiconductor (FMSs), InFeAs, GaFeSb, InFeSb, are promising materials, because Fe atoms are in the neutral state thus do not supply carriers but only local spins in III-V semiconductors, so we can realize both n and p-type and their Curie temperatures can be over room temperature [1,2]. Meanwhile, InAs / GaSb heterostructures have some novel properties; staggered bands, little lattice mismatch (~0.6%), and high electron mobility. In the heterostructure of an InAs quantum well with a GaFeSb barrier, the in-plane transport shows the unique magnetoresistance (MR) originated from the scattering of *s* electrons in InAs as a non-ferromagnet layer with *d* electrons from the magnetization of GaFeSb at the InAs/GaFeSb interface. Note that the resistance of InAs is much lower than that of GaFeSb by more than two orders of magnitude. Therefore, the carriers flow only in the InAs layer. In this study, we observe this MR and modulate it by applying a gate voltage.

We have grown InAs (15 nm) / GaFeSb (15 nm, Fe 20%) / AlSb (300 nm) / AlAs (15 nm) / GaAs (100 nm) on semi-insulating GaAs (001) substrates by low temperature molecular beam epitaxy (Fig. 1(a)). This sample was patterned into a 100 x 200 μm^2 Hall bar; HfO₂ was deposited for a gate insulating layer by atomic layer deposition; the Au gate electrode was fabricated (Fig. 1(b)). In the measurement, we applied the gate voltage from the gate pad to the source electrode and measured the MR by the four terminal method.

Figure 1(c) shows the magnetic field H ($= 1$ T) angle direction dependence of the resistance when the current $J_{DS} = 4.3 \mu\text{A}$ and the gate voltage $V_g = 0$ V at 3.5 K. H was rotated (in the *y-z* plane) as it was always perpendicular to J_{DS} ($// x$ axis), and $\theta = 0^\circ$ and 90° means perpendicular to the film plane and in the film plane, respectively. The MR ratio is 2.7%, which is large compared with another study about the in-plane transport of ferromagnet / non-ferromagnet [3][4]. This result means that the electron wavefunction in the InAs penetrates into the GaFeSb even at $V_g = 0$ V and it is the origin of the anisotropy of the MR. Then, we applied V_g and the MR ratio reaches 7.8% when $V_g = -3$ V. We can successfully control the electron wavefunction and enhance

the MR in the InAs/GaFeSb heterostructure. In addition, the J_{DS} vs. source-drain voltage V_{DS} shows the transistor behavior, which means J_{DS} is greatly modulated by V_g , and

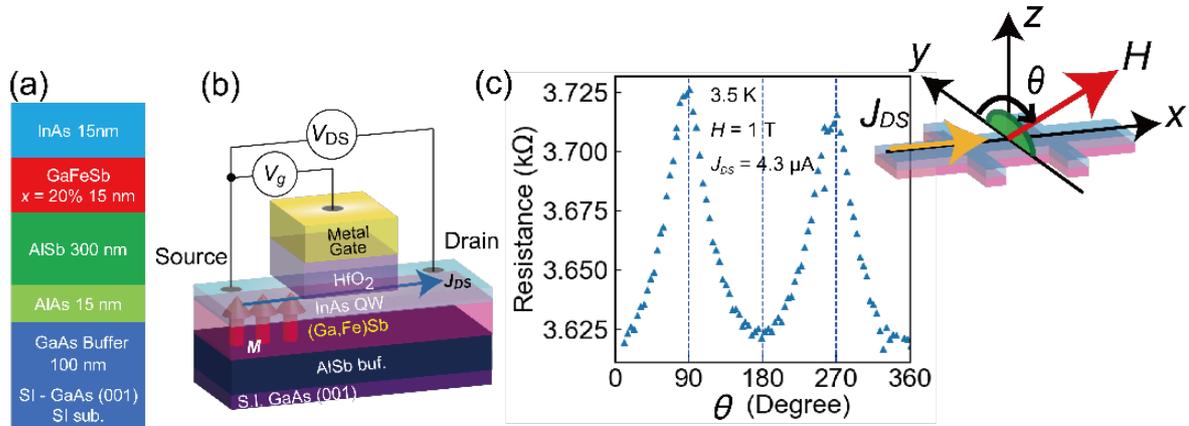


Figure 1 Schematic (a) sample. and (b) device structure with the gate electrode.

(c) Magnetic field direction dependence of the resistance when $V_g = 0$ V.

finally we confirmed that this device behaves like a magnetic transistor.

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Spatial distribution of substitutional Mn-As clusters in ferromagnetic (Zn,Sn,Mn)As₂ thin films revealed by image reconstruction of atom probe tomography

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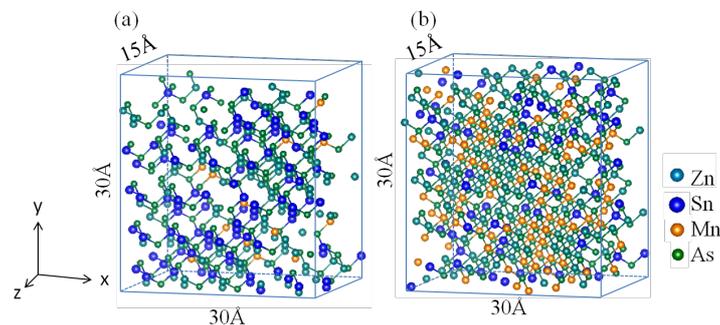
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Ferromagnetic transition in (Zn,Sn,Mn)As₂ thin films is explained by magnetic percolation with Mn-As clustering network [1]. We studied the spatial relationship of Mn-As clusters with the resulting Curie temperature (T_C) in the materials, assuming the reconstruction of local atomic structures from dataset of atomic positions in (Zn,Sn,Mn)As₂ obtained by atom probe tomography (APT). To probe local atomic structures and magnetic properties of Mn-As cluster in ZnSnAs₂ thin films, we investigated (Zn,Sn,Mn)As₂ samples doped with 2.1 and 3.6 at. % Mn, which were grown on (001) InP substrates by molecular beam epitaxy. Several representative regions with low and high Mn concentration were extracted from APT dataset. Mn-As clusters consisting of 2 - 36 Mn-As cluster configurations in the reconstructed local structures of high Mn concentration regions were identified. We also obtained a correlation between T_C and Mn-As clustering consistent not only with the experimental results but also with the first principles calculation using mean-field approximation.



Reconstruction lattice of (a) low Mn concentration region and (b) high Mn concentration region. The atomic positions are determined on the assumption of a sphalerite structure with lattice parameters of $a = 5.85$, $b = 5.85$, and $c = 11.7$ Å.

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No. 08

A first-principles study on the magnetism of Fe/Bi/MgO multilayers

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The magnetic tunnel junction (MTJ) has a structure consisting of two ferromagnetic layers separated by a thin insulating layer. MTJ is used for the magnetoresistive random access memory (MRAM) cell with giant magneto resistance ratio. MRAM is a nonvolatile memory without requiring standby power to keep information and has attracted much attention as a new generation of low power consumption memory. Strong perpendicular magnetic anisotropy to realize high density memory devices is highly desired for preventing thermal magnetic fluctuation in the ferromagnetic layer of MTJ. Perpendicular magnetic anisotropy originates from magnetocrystalline anisotropy (MCA) caused by spin-orbit coupling. In this study, we investigate the influence of a Bi layer insertion at Fe/MgO interface by first-principles density-functional calculations. We first propose models of Fe/Bi/MgO by considering lattice matching for the calculations and then study the magnetism of Fe/Bi/MgO as well as Fe monolayer and Fe/MgO films. It is found that enhancement in perpendicular magnetic anisotropy can be obtained by inserting the Bi layer at the Fe/MgO interface. The electronic origin of MCA in the systems is discussed from the viewpoint of Bruno's formula [1] and band structure within the second-order perturbation theory [2].

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Growth of Fe₄N films toward fabrication of Fe₄N-based current-perpendicular-to-plane giant magnetoresistance devices

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Anti-perovskite type 3d transition metal ferromagnetic nitrides are a promising candidate as a new spintronics material. Fe₄N, one of these compounds, is theoretically predicted to have a large negative spin-polarization of electrical conductivity ($P_s = -1.0$) [1]. In addition, large tunnel magnetoresistance effect is theoretically expected due to coherent tunneling in the Fe₄N/MgO/Fe₄N magnetic tunnel junction with perpendicular magnetic anisotropy [2], and voltage control of magnetocrystalline anisotropy in Fe₄N/MgO is predicted by theoretical calculations [3]. On the other hand, we consider that the large $|P_s|$ and relatively high electrical resistivity of Fe₄N is suitable for application to a current-perpendicular-to-plane giant magnetoresistance (CPP-GMR) recording head of a next generation hard disk drive [4]. In this work, we grew Fe₄N epitaxial films by molecular beam epitaxy toward fabrication of Fe₄N-based CPP-GMR devices.

The Fe₄N film was grown on SrTiO₃(STO)(001) substrates at 500 °C by supplying Fe and radio-frequency N₂ plasma, simultaneously. Figures 1 and 2 show the reflection high-energy electron diffraction (RHEED) and out-of-plane x-ray diffraction (XRD) patterns of the Fe₄N film, respectively. Epitaxial growth of the Fe₄N film on the STO(001) substrate was confirmed. As a next step, we try to grow Fe₄N films on a metallic buffer layer, and Fe₄N/non-magnetic metal/Fe₄N tri-layer structure.

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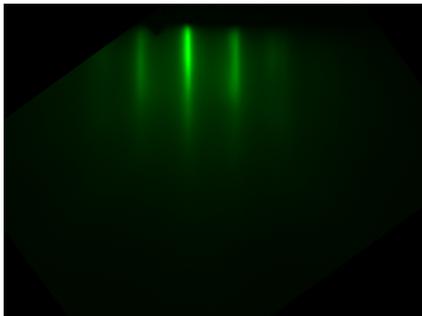


Fig. 1 RHEED pattern of the Fe₄N layer.

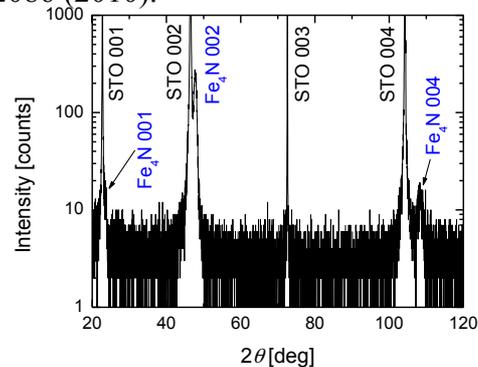


Fig. 2 Out-of-plane XRD pattern of the sample.