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Unitarity in gauge symmetry breaking on orbifold. Y. Abe, N. Haba, Y. Higashide, K. Kobayashi, M. Matsunaga: Progress of Theoretical Physics, 109, pp.831 - 842, 2003.

We study the unitarity bounds of the scattering amplitudes in the extra dimensional gauge theory where the gauge symmetry is broken by the boundary condition. The estimation of the amplitude of the diagram including four massive gauge bosons in the external line shows the power behavior of the amplitude is canceled. The calculation will be done in the 5 dimensional standard model and the SU(5) grand unified theory, whose 5th dimensional coordinate is compactified on S^1/Z_2. The broken gauge theories through the orbifolding preserve the unitarity at high energies similarly to the broken gauge theories where the gauge bosons obtain their masses through the Higgs mechanism. We show that the contributions of the Kaluza-Klein states play the crucial rolls for conserving the unitarity.

Correlation Functions at Antiferroelectric Smectics by Means of Transfer Matrix Method, S. TANAKA* and M. YAMASHITA: Mol. Cryst. Liq. Cryst. 398, pp. 45-56, 2003.

The mechanism of successive phase transitions occurring at antiferro-electric smectics is well described by ANNNI model. Here the transfer matrix method is generalised so as to be applied to this model with long range interaction. The correlation function is obtained, which shows oscillating behaviour with varying wave number due to the complex eigenvalue of transfer matrix. In the framework of this method the critical temperature of the model is estimated by replacing an intralayer interaction by the molecular field.

Maier-Saupe Nematic Isotropic Phase Transition in the Presence of an External Field, M. Yamashita: Mol. Cryst. Liq. Cryst. 398, pp. 75-85, 2003.

The nematic-isotropic phase transition in an external field is studied in the frame of Maier-Saupe model, where a global phase diagram including both cases of positive and negative susceptibility anisotropic is obtained. In the extreme case of infinitely large negative anisotropy, the system is reduced to the classical XY model because the rotational degree of freedom is restricted to lie in the plane perpendicular to the field, in which the second order phase transition occurs. The crossover of the directional degree of freedom between 3-dimension and 2-dimension is depicted. On the other hand, the critical point appears at a certain strength of the positive anisotropy, beyond which the transition disappears. The theory can be applied to the phase transition of very thin systems with homeotropic and planar anchorings.

Global Phase Diagram of Maier-Saupe Model and Inhomogeneity Due to Walls, M. Yamashita: J. Phys. Soc. Jpn. 72, pp. 1682-1688, 2003.

A global phase diagram of Maier-Saupe model for nematic-isotropic phase transition on the external field versus temperature plane is obtained, where due to non-polar property of the system two sets of order parameters and the conjugate fields are required to describe completely the phenomena. The phase diagram is argued in the context of a similarity of the model to the three-state Potts model. Inhomogeneity at the thin system sandwiched by parallel walls is expressed in terms of an effective external field, where effects due to homeotropic, homogeneous, planer and oblique anchoring walls are classified systematically. A shift of the transition temperature together with the property of phase transition is explained systematically on the basis of the phase diagram of bulk system, where the changes of the order of phase transition is related to a critical point and a tricritical one appearing in the phase diagram.

Continuous Phase Change Mediated by an Unstable State at Freely Suspended Smectic Films, M. Yamashita: J. Phys. Soc. Jpn. 72, pp. 2421-2424, 2003

Phase transitions of freely suspended chiral smectic films exhibiting a first order phase transition in a bulk system are studied in the framework of a phenomenological theory, in which such a widely observed finding that the surface layer orders at a temperature higher than the bulk critical temperature is taken into account. While the inner portion of the film exhibits the first order phase transition at a temperature below that of the surface layer in the system of sufficient thickness, a continuous change occurs for the system with a thickness smaller than a critical thickness. The mechanism of the continuous change is elucidated on the basis of the phase diagram of the bulk system on the field versus temperature plane, where nonuniformity due to the ordered surface layers is replaced by an effective field and the high-temperature phase is connected

Unambiguous relationship between the Hubbard, t-J and d-p models in One-dimension based on the Luttinger liquid Theory, Kazuhiro Sano and Yoshiaki Ono*: Physica C388-389., pp. 84-85, 2003.

We examine the one-dimensional (1D) d-p model in comparison with typical 1D models such as the 1D Hubbard model and the 1D t-J model using the numerical diagonalization method combined with the Luttinger liquid theory. We calculate the spin velocity $v\sigma$, the charge velocity $v\rho$ and the Luttinger liquid parameter $K\rho$ for each model. Using these parameters, a relationship between the models is obtained unambiguously. We find that the d-p model can be described by the Hubbard model in the wide parameter region, while it can be described by the t-J model only in the strong coupling limit.

Ferromagnetism and Superconductivity in the Multi-orbital Hubbard Model: Hund's Rule Coupling versus Crystal-Field Splitting, Kazuhiro Sano and Yoshiaki Ono*: J. Phys. Soc. Jpn, 72, pp. 1847-1850, 2003.

The multi-orbital Hubbard model in one dimension is studied using the numerical diagonalization method. Due to the effect of crystal-field splitting Δ, the fully polarized ferromagnetism, which is observed in the strong coupling regime, becomes unstable against the partially polarized ferromagnetism when Hund's rule coupling J is smaller than a certain critical value of order of Δ. In the vicinity of the partially polarized ferromagnetism, the orbital fluctuation develops due to the competition between Hund's rule coupling and crystal-field splitting. The superconducting phase with the Luttinger liquid parameter $K\rho$ is observed for the singlet ground state in this region.

Nonlinear Sigma model method for the J1-J2 Heisenberg model: disordered ground state with plaquette symmetry, K. Takano, Y. Kito, Y. Ono, K. Sano: Phys. Rev. Lett. 91, pp.197202-1-197202-4 , 2003.

A novel nonlinear model method is proposed for the two-dimensional J1-J2 model which is extended to include plaquette-type distortion. The nonlinear model is properly derived without spoiling the original spin degrees of freedom. The method shows that a single disordered phase continuously extends from a frustrated uniform regime to an unfrustrated distorted regime. By the continuity and Oshikawa’s commensurability condition, the disordered ground states for the uniform J1-J2 model are plaquette states with fourfold degeneracy.

Semigrand Canonical Monte Carlo Simulation with Gibbs-Duhem Integration Technique for Alloy Phase Diagram, Atsushi MORI*, Brian B. LAIRD*, Yoshihiro KANGAWA*, Tomonori ITO and Akinori Koukitu*: Materials Physics and Mechanics, 6, pp.49 - 57, 2003.

Formulation is given for the Gibbs-Duhem integration (GDI) method in the semigrand canonical (SGC) ensemble, in which the total number of particles N is fixed with the specified chemical potential differences between species $\Delta\mu$. Demonstration of the SGC Monte Carlo simulation with the GDI technique is given for a pseudo-binary semiconductor alloy $In_xGa_{1-x}N$.

Semigrand Canonical Monte Carlo Simulation with Gibbs-Duhem Integration Technique: Formulation for Alloy Phase Diagrams and Attempt on $In_xGa_{1-x}N$/GaN, Atsushi MORI*, Brian B. LAIRD*, Yoshihiro KANGAWA*, Tomonori ITO and Akinori KOUKITU*: Russian Journal of Physical Chemistry, 77, pp.521-529, 2003.

We give formulation for the Gibbs-Duhem integration (GDI) method in the semigrand canonical (SGC) ensemble, in which the total number of particles N is fixed with the specified chemical potential differences between species $\Delta\mu$. For a binary system in the isobaric SGC ensemble, the equation to be integrated in the T-$\Delta\mu$ plane is $d(\Delta\mu^{eq})/dT=-\Delta h/T\Delta x$, where $\Delta\mu^{eq}$ gives $\Delta\mu$ at equilibrium between phases I and II at temperature T, Δh represents enthalpy difference h^{II}-h^{I}, and Δx represents the composition differences x^{I}-x^{II}. Attempting application of SGC Monte Carlo simulation with the GDI technique to a pseudobinary semiconductor alloy $In_xGa_{1-x}N$ is presented, the preliminary result of which reflects the asymmetric nature of an excess energy curve calculated on the basis of an empirical interatomic potential used in the present Monte Carlo simulation.

Intra-Atomic Noncollinear Magnetism and the Magnetic Structures of Antiferromagnetic FeMn, Kohji NAKAMURA, Tomonori ITO, A. J. FREEMAN*, Lieping ZHONG* and J. Fernandez-de-CASTRO*: Physical Review B, 67, pp. 014405-1-4, 2003.

Both collinear and noncollinear magnetic structures of FeMn with $L1_0$ atomic ordering were determined from total-energy full-potential linearized augmented plane-wave calculations incorporating noncollinear magnetism with no shape approximation for the magnetization density. Different spin-density orientations for the different band states are observed on a smaller length scale inside an atom. The presence of the intra-atomic noncollinear magnetism enhances the stability of the 3Q noncollinear magnetic structure, in which the magnetic moments align toward the center of the cell of four atoms, thus becoming the lowest-energy state of the structures considered.

Enhancement of Magnetocrystalline Anisotropy in Ferromagnetic Fe Films by Intra-Atomic Noncollinear Magnetism, Kohji NAKAMURA, Tomonori ITO, A. J. FREEMAN*, Lieping ZHONG* and J. Fernandez-de-CASTRO*: Physical Review B, 67, pp. 014420-1-6, 2003.

We generalize the full-potential linearized augmented plane-wave method with a single slab geometry in order to treat noncollinear magnetism with no shape approximation for the magnetization, and apply this scheme investigate free-standing Fe(001) monolayers with lattice constants matching those of fcc Ag(001) and Cu(001) substrates. Intra-atomic noncollinear magnetism on a smaller length scale inside the atom is observed in the ferromagnetic state, and is found to enhance the magnetocrystalline anisotropy energy (by 17~20%) compared to values determined for their collinear magnetic state.

First Principles Investigation of Domain Walls and Exchange Stiffness in Ferromagnetic Fe and Antiferromagnetic NiMn, Kohji NAKAMURA, Tomonori ITO, A. J. FREEMAN*, Lieping ZHONG* and J. Fernandez-de-CASTRO*: Journal of Applied Physics, 93, pp. 6879-6881, 2003.

We investigate the domain walls in ferromagnetic Fe and antiferromagnetic NiMn with the first principles full-potential linearized augmented plane-wave method including intra-atomic noncollinear magnetism. In both cases, the self-consistent results demonstrate that the magnetization changes continuously from one orientation to another as seen in a Bloch wall. The formation energy of the domain wall significantly decreases when the wall thickness increases, which leads to an exchange stiffness of 1.13×10^{-11}J/m for Fe and 1.43×10^{-11}J/m for NiMn. The predictions agree with those determined separately for Fe from a phenomenological calculation

Curling Spin Density and Orbital Structures in a Magnetic Vortex Core of an Fe Quantum Dot, Kohji NAKAMURA, Tomonori ITO and A. J. FREEMAN*: Physical Review B, 68, pp. 180404(R)-1-4, 2003.

First results of the spin and orbital structures in the vortex core of an Fe dot obtained using highly precise first principles calculations that include intra-atomic noncollinear magnetism are reported. We demonstrate that a curling magnetic structure is stabilized within a 4 nm radius dot as inferred from spin-polarized scanning tunneling microscopy experiments in which the spin directions close to the center of the dot turn up along the perpendicular orientation to the curling plane-and also predict a complicated curling intra-atomic noncollinear magnetism near the center in which the spin moments continuously cant in circular directions on a smaller length scale inside the atoms. Importantly, these rotation properties in the spin density couple to the orbital motion and induce orbital moments oriented perpendicular to the curling plane, which is a first prediction of quantum phenomena induced in the nanoscale vortex core.

Influence of lattice Constraint from InN and GaN Substrate on Relationship between Solid Composition of $In_xGa_{1-x}N$ Film and Input Mole Ratio during Molecular Beam Epitaxy, Yoshihiro KANGAWA*, Tomonori ITO, Yoshinao KUMAGAI*, Akinori KOUKITU* and Norihito KAWAGUCHI*: Japanese Journal of Applied Physics, 42, pp. L95-L98, 2003.

Thermodynamic analyses were carried out to understand the influence of lattice constraint from InN and GaN substrates on the relationship between solid composition x of $In_xGa_{1-x}N$ films and input mole ratio R_{In}. The calculation results suggest that a compositionally unstable region is found at the GaN-rich region for InGaN on InN at higher temperatures while that for INGaN on GaN can be seen at the InN-rich region. This is because the maximum enthalpy of mixing shifts toward x~0.10 for InGaN on InN and toward x~0.80 for InGaN on GaN compared with x~0.50 for stress-free InGaN.

Effect of Ni-Cu Substrates on Phase Selection of Hexagonal and Cubic Boron Nitride Thin Films, Shigeo KOTAKE, Takaya HASEGAWA, Kazutaka KAMIYA, Yasuyuki SUZUKI, Takami MASUI*, Yoshihiro KANGAWA*, Kohji NAKAMURA and Tomonori ITO: Applied Surface Science, 216, pp. 72-77, 2003.

The dependence of the phase selection of BN on the lattice parameter and the crystal structure of the substrate was clarified. BN thin films were prepared by RF sputtering method on polycrystalline Ni-Cu complete solid solution alloy. Using empirical potentials, the polytypes of BN thin films were systematically investigated by considering lattice constraint due to various interface atomic arrangements and orientations such as c-BN or h-Bn on cubic (001) or (111) substrates. From IR spectrum, merely c-BN phase was observed from the specimen on Cu and $Ni_{0.8}$-$Cu_{0.2}$ alloy. Moreover, the empirical potential calculations reveal that c-BN thin films on (001) substrates can be stabilized in the substrate lattice parameter of $3.2<a<4.4$ Å.

Thermodynamic Study on Compositional Instability of InGaN/GaN and InGaN/InN during MBE, Yoshihiro KANGAWA*, Tomonori ITO, Yoshinao KUMAGAI* and Akinori KOUKITU*: Applied Surface Science, 216, pp. 453-457, 2003.

Thermodynamic analyses were carried out to understand the influence of lattice constraint from GaN and InN substrates on relationship between solid composition x of $In_xGa_{1-x}N$ films and input mole ratio R_{In}. The calculated results suggest that a compositional unstable region is found at small R_{In} region for InGaN on InN while that for INGaN on GaN can be seen at large R_{In} region at higher temperatures. This implies that InN-rich thin films are possible to form on InN substrate though it is difficult to form on GaN substrate.

Systematic Theoretical Investigations of Miscibility in $Si_{1-x-y}Ge_xC_y$ Thin Films, Tomonori ITO, Kohji NAKAMURA, Yoshihiro KANGAWA*, Kenji SHIRAISHI*, Akihito TAGUCHI* and Hiroyuki KAGESHIMA*: Applied Surface Science, 216, pp. 458-462, 2003.

Miscibility of C in $Si_{1-x-y}Ge_xC_y$ thin films is systematically investigated by using the empirical interatomic potentials. The empirical potential approach is applied to calculate excess energies for $Si_{1-x-y}Ge_xC_y$ thin films incorporating interface lattice constraint due to Si(001). In order to compare with experimental results, we employ the content values such as x=0.13, 0.22, 0.27, 0.31, 0.35, and y=0.019. The calculated results imply that the lattice constraint at the interface and Si-C interatomic bond formation dramatically reduce excess energies of $Si_{1-x-y}Ge_xC_y$ thin films by 20-30% of those in bulk state. Therefore, the lattice constraint promotes C incorporation in $Si_{1-x-y}Ge_xC_y$ thin films. Furthermore, segregation phenomena of Ge and C atoms in $Si_{0.78}Ge_{0.2}C_{0.02}$ on Si(001) is clarified by Monte Carlo simulation taking into account surface and interface structures. The simulated results reveal that Ge atoms segregate in the topmost layer and C atoms accumulate in the second layer.

An Empirical Potential Approach to Structural Stability of GaN_xAs_{1-x}, Takashi SUDA, Yoshihiro KANGAWA*, Kohji NAKAMURA and Tomonori ITO: Journal of Crystal Growth, 258, pp. 277-282, 2003.

Thermodynamic stability of GaN_xAs_{1-x} including zinc blende (ZB) – wurtzite (W) structural stability and miscibility is systematically investigated based on a newly developed empirical potential, which incorporates electrostatic energies due to bond charges and ionic charges. Using the empirical potential, the system energies of W and ZB form are calculated for bulk GaN_xAs_{1-x} over the entire concentration range. The calculated results predict that the structural phase transition from ZB to W occurs at x~0.4, which differs from x~0.7 estimated by electrostatic energy contributions. The shift of the ZB-W structural transition concentration toward x~0.4 is clarified in terms of difference in bond length distribution between ZB- and W-GaN_xAs_{1-x}. Based on these findings, the miscibility of GaN_xAs_{1-x} is discussed by excess energy calculations.

Atomic and Electronic Structure of Misfit Dislocations in GaSb/GaAs(001), Nori MIYAGISHIMA*, Takuya SHINODA*, Ken SUZUKI*, Tadasuke KANEKO*, Kyozaburo TAKEDA*, Kenji SHIRAISHI* and Tomonori ITO: Phyisica B, 340-342, pp. 1009-1012, 2003.

We investigated the atomic and electronic structures of the periodic misfit dislocations (MDs) found in GaSb/GaAs(001). In order to determine the details of these structures, we carried out the first-principle total energy calculations. The characteristic feature in the MDs is the appearance of the anion-anion or cation-cation bond in order to avoid the formation of dangling bonds. As a result, the dislocation core structure form five- and seven-membered rings. These MDs electronically cause the impurity levels in the band gap. The individual MDs have the possibility to form one-dimensional electron- and hole-paths along the dislocation line.

Superlattice Stacking Structure in InGaN Thin Film Pseudomorphic to GaN(0001) Substrate: Semigrand Canonical Monte Carlo Simulation, Atsushi MORI*, Tomonori ITO, Yoshihiro KANGAWA*, Yoshinao KUMAGAI* and Akinori KOUKITU*: Physica Status Solidi (c), 0, pp. 2486-2489, 2003.

Superlattice stacking structures in the Ga-rich branch of wurtzite $In_xGa_{1-x}N$/GaN were found using semigrand canonical Monte Carlo simulations, which were performed aiming at the construction of the alloy phase diagram. Simulated systems were $In_xGa_{1-x}N$ thin films pseudomorphic to the GaN(0001) substrate. Continuing the simulations, we revealed that In-rich layers parallel to the substrate were formed in Ga-rich regions. At 800 K, traversing along the *c* direction GGGIGGGI… superlattice-type stackings were more frequently observed, where G and I indicate the Ga-rich and In-rich layers, respectively. As the temperature increased along the two-phase boundary the superlattice structure changes so that many In-rich layers were included. The In content of the Ga-rich phase eventually exceeded 0.5 at a higher temperature such as 875 K.

Influence of Lattice Constraint from InN and GaN Substrate on Relationship between Input Mole Ratio and Solid Composition of InGaN during MOVPE, Yoshihiro KANGAWA*, Tomonori ITO, Yoshinao KUMAGAI* and Akinori KOUKITU*: Physica Status Solidi (c), 0, pp. 2575-2579, 2003.

Thermodynamic analyses incorporating the contribution of lattice constraint from the substrates were carried out to understand the relationship between input In mole ratio and solid composition of stress-free InGaN, InGaN on GaN and InGaN on InN during metalorganic vapor phase epitaxy. The calculated results suggest that a compositionally unstable region is found at the InN-rich region for InGaN on GaN at high temperatures, while that for InGaN on InN can be seen at the GaN-rich region due to the lattice constraint from the substrate. These results imply that incorporating the contribution of lattice constraint is indispensable to predict the thermodynamic properties of such materials.

Influence of Lattice Constraint from Substrate on Relationship between Input Mole Ratio and Solid Composition of InGaN during MBE and MOVPE [in Japanese], Yoshihiro KANGAWA*, Tomonori ITO, Yoshinao KUMAGAI* and Akinori KOUKITU*: Journal of the Japanese Association for Crystal Growth, 30, pp.104 - 110, 2003.

Thermodynamic analyses were performed to understand the influence of lattice constraint from InN and GaN substrates on the relationship between solid composition x of $In_xGa_{1-x}N$ films and input mole ratio R_{In} during molecular beam epitaxy (MBE) and metalorganic vapor phase epitaxy (MOVPE). For the both growth methods, the calculation results suggest that a compositionally unstable region is found at the InN-rich region for InGaN on GaN at higher temperatures while that for InGaN on InN can be seen at GaN-rich region due to the lattice constraint from the substrate. Incase of the MOVPE, it is found that growth region of InGaN in the diagram related to V/III ratio and solid composition shrinks with increase of V/III ratio. This is because the H_2 partial pressure produced by the decomposition of NH_3 increase at high V/III ratio

Ab initio-Based Approach to Structural Stability of GaAs Surfaces [in Japanese], Yoshihiro KANGAWA*, Tomonori ITO, Kenji SHIRAISHI*, Tadashi OHACHI and Akinori KOUKITU: Journal of the Surface Science Society of Japan, 24, pp. 642-647, 2003.

An *ab initio*-based approach was made to understand the influences of temperature and beam equivalent pressure (BEP) on the structural stability of GaAs surfaces. The theoretical approach incorporates free energy of vapor phase; therefore we can calculate how structural stability of GaAs surfaces depends on the temperature and beam equivalent pressure. By the theoretical investigations, temperature and BEP dependencies of the stability of GaAs(001)-(4x2) were predicted. The results agree with experimental results, and feasibility of the theoretical approach was confirmed. Furthermore, the relative stability of Ga adatom among the case of that on GaAs(001)-(2x4) and (11*n*)A (n=2, 3, 4) surfaces were studied.

First-principles Study of Reaction of Atomic Oxygen at SiO_2/Si(100) Interface, Toru AKIYAMA and Hiroyuki KAGESHIMA*: Proc. of the 26th International Conference on the Physics of Semiconductors, Edinburgh, 2003.

Structures, energetics, and reaction kinetics of atomic oxygen at SiO_2/Si(100) interfaces are investigated based on total-energy electronic-structure calculations within the density functional theory. It is found that oxygen atoms in the oxide region form Si-O-O-Si bonds, whereas Si-O-Si bonds are formed in the substrate. It is also found that the reaction of atomic oxygen is largely exothermic. A possible reaction mechanism for atomic oxygen is suggested from obtained structures.

Origin of Interfacial Reaction Constant for Si Thermal Oxidation, Toru AKIYAMA and Hiroyuki KAGESHIMA*: Extend abstracts of the 2003 International Conference on Solid State Devices and Materials, Tokyo, pp. 490-491, 2003.

We present first-principles calculations that clarify mechanisms of reaction of oxygen molecules at SiO2/Si(100) interface. The energy barriers for the reaction of oxygen at the interface corresponds to the floating bond formation process between the oxygen of oxidant and the host Si atom at the interface, and agree well with the experimentally reported activation energies for ultrathin oxide. The present results imply that the accumulation of strain induced by oxidation crucially affect the interfacial reaction. It is indicated that the origin of the activation energy of the reaction constant B/A in the Deal-Grove model due to this effect.

Microscopic Behavior of Atomic Oxygen at the SiO_2/Si(100) Interface [in Japanese], Toru AKIYAMA and Hiroyuki KAGESHIMA*: Extend abstracts of the 8-th Workshop on Formation, Characterization, and Reliability of Ultrathin Silicon Oxides, pp. 273-277, 2003.

The atomic process of oxygen atom near the SiO_2/Si(100) interface is studied based on total-energy electronic-structure calculations. The calculations of O atoms in SiO_2 indicate that O atoms diffuse by changing Si-O-O-Si bond (peroxy linkage configuration) without forming isolated O atom configuration. It is found that calculated energy barriers for this mechanism are in the range of 0.6-1.0 eV. The energies of Si-O-Si bond at the top of Si substrate are much lower than those of O atom in SiO_2. The result indicates that the reaction in which an O atom in the oxide incorporated in the substrate is largely exothermic. It is also found that the calculated energy barrier for this reaction is lower than the experimentally reported activation energy for the interfacial reaction process in the dry oxidation. Detailed investigation for the atomic process of interfacial reaction is thus important for the interpretation of experimentally reported activation energy.

Microscopic Mechanism of Interfacial Reaction during Si Oxidation, Toru AKIYAMA and Hiroyuki KAGESHIMA*: Applied Surface Science 216, pp. 264-268, 2003.

The reaction of atomic oxygen at the SiO_2/Si(100) interface is studied based on total-energy electronic-structure calculations. It is found that the reaction in which an O atom in the oxide inserts into the Si-Si bond of the substrate is largely exothermic. The calculated energy barrier of 0.87 eV for this reaction is lower than the experimentally reported activation energy (2.0 eV) for the interfacial reaction in the dry oxidation. The results would help us clarify the microscopic mechanism of Si oxidation, especially in identifying the form of oxidant in the dry oxidation.

Dependence of the Magnetic Properties of TbFeCo Films on the Species of Sputtering Gases Used, Masahito MORIMOTO, Tomohiro INAGAKI, Tadashi KOBAYASHI, Yuji FUJIWARA, Morio MASUDA, Shigeru SHIOMI and Tsutomu SHIRATORI*: J. Magn. Soc. Jpn., 27, pp.269-272, 2003.

This paper investigates what the magnetic characteristics of TbFeCo films would become if Ar and Kr were used as sputtering gases. The sample structure was glass / underlayer SiN_x(u) / TbFeCo / protective layer SiN_x(p), and the top three layers were deposited by magnetron sputtering. When Kr gas was used, the coercive force H_c and effective perpendicular anisotropy K_{eff} increased. The increase was not dependent on the difference in Curie temperature. The type of sputtering gas used was changed for deposition of the SiN_x(u) and TbFeCo layers. Consequently, H_c increased when TbFeCo was deposited by using Kr gas. Changing the kind of sputtering gas used seldom affected SiN_x(u).

Magnetoresistance Effect of Co/AlO[x]/NiFe/Au/n-Si Diode Structure, Y. Fujiwara, T. Hirose, M. Jimbo, T. Kobayashi, M. Masuda, Jpn. J. Appl. Phys. 42, pp L1009-L1011, 2003.

Magnetoelectronic properties were investigated for a Co/AlOx/NiFe/Au/n-Si diode structure utilizing the two-point-probe method at 77 K. In this system, electrons were transported from the Co layer to the n-Si substrate through the AlOx tunneling barrier, NiFe magnetic layer and Au/n-Si Schottky barrier. When a positive bias (a reverse bias to Au/n-Si Schottky diode) was applied between Co and n-Si, the current slightly increased with increasing positive bias voltage up to approximately 0.75 V, and abruptly increased at a positive bias voltage over 0.75 V. The observed current showed a large magnetoresistance effect of approximately 600%.

Material Processing Using Microorganisms (An Investigation of Microbial Action on Metals), Yasushi KUROSAKI, Masahito MATSUI, Yuichi NAKAMURA, Kenichi MURAI and *Toshio KIMURA: JSME International Journal, Series C, Vol. 46, No. 1, pp. 322-330, 2003.

The possibilities for developing a new type of material processing using a microbiogenic function are investigated with a microbial corrosion test of metals under the sea water. The behavior of microorganisms in the corrosion of metals (mild steel, copper and aluminum sheets) is examined, and their action on these metals is discussed. As a result, three processing methods (biomachining, biodeposition and biorecycling) are proposed and discussed.

Oxygen Partial Pressure Dependences of a-c Phase Ratio, Crystallinity, Surface Roughness and In-Plane Orientation in YBCO Thin Film Depositions by IBS, T. Endo, K Yoshii, S. Iwasaki, H. Kohmoto, H. Saratani, S. Shiomi, M. Matsui and Y. Kurosaki: Proceedings of IUMRS International Conference on Electronic Materials (Xi'an 2002); Superconductor Science and Technology, Vol. 16, pp.110-119, 2003.

$YBa_2Cu_3O_X$ thin films were grown on MgO by ion beam sputtering at various substrate temperatures T_S and oxygen partial pressures P_O with a supply of either oxygen molecules or plasma (PL) to study fundamental crystal growth of perovskite oxide. The *a*-phase growth is enhanced by PL due to two mechanisms, the collision retarded surface migration, and plasma energy assisted atomic rearrangement and surface energy reduction. The mixed film can release a strain energy from interior grain to ambient media, then it has good crystallinity but a rough surface. In contrast, the pure single *a*-phase film has poor crystallinities but the smoothest surface because the strain energy is stored in the interior. In-plane orientation is improved by increasing the *a*-phase ratio, and in-plane crystallinity can be improved by PL.

Quantitative Estimation of Fracture Surface for Mild Steel Using Fractal Analysis, Mir Behdad KHAMESEE, Masahito MATSUI, Kenichi MURAI, *Toshihide ISHIHARA and Yasushi KUROSAKI: Proceedings of the IMMM2003, pp.147-152, 2003.

The use of fractal dimension calculations, for quantitative classification of various objects, is well established in many areas of the physical and life sciences. Such fractal dimension calculations are useful in that they furnish some measure of geometrical complexity that is not available through traditional approaches. In this research fractal analysis was applied for quantitative estimation of fracture surfaces. Fracture surface profiles of mild steel were generated under various kinds of notch root (shape and radius) and tensile speed tests are examined by employing two methods of fractal analysis. A method for quantitative estimation of fracture surface phenomenon caused by fracture accidents is presented, and its validity is confirmed. Although the fractography has used for texture determination of fracture surfaces, it is known that the surface fractography is not enough for quantitative estimation of fracture surface but it is necessary. Even if under the same fracture type, fractal dimension is not constant, but depends on the specimen shape, and thus on the fracture strain. By using fractal dimension and fractography as a method, fracture surface can be estimated.

Micro-Rheometry of Pressurized Lubricants and Micro-Nanorheology, Yuichi NAKAMURA and Yasushi KUROSAKI, Proc. 2003 JSME-IIP/ASME-ISPS Joint Conference on Micromechatronics for Information and Precision Equipment, pp.69-70, 2003.

In the present study, micro-rheometry of pressurized lubricants employing a diamond-anvil pressure cell and a laser confocal displacement sensor of 0.4μm resolution was shown.. High pressure viscosity was obtained up to 2 GPa at 200 ℃ for traction oils and PFPE oils. The linearity between logarithmic viscosity and pressure is confirmed. Viscosity-pressure coefficient α at room temperature was almost twice larger than that at 100 ℃. α for hard disk oil, Zdol2000, was 13 /GPa at 24 ℃ ～ 5 /GPa at 150 ℃and was similar to that of paraffinic mineral oil. The feature of the obtained high pressure volume was different for each oil up to 6 GPa. Zdol2000 was the most compressible of all the sample lubricants and its high pressure refractive index increased about 10 % at 4.8 GPa. Zdol2000 remained transparent up to 4.8 GPa under isothermal loading. Some considerations for lubricant's micro-nanorheology was also mentioned with high pressure lubricant's rheology.