

Department of Physics Engineering

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Fluctuation Spectrum of Director in Cholesteric Phase with External Field, M. Yamashita: *Mol. Cryst. Liq. Cryst.* 409, pp. 219-227, 2004.

Fluctuation spectrum of molecular orientation in the cholesteric phase exposed to the external field with positive anisotropy is calculated for the general case of Frank's elastic constants. The stability of the phase is certified in the meaning of Peierls-Landau theory.

The Order and the Polarisation of the System Composed of Polar Gay-Berne Molecules with Bend, T. Miyazaki* and M. Yamashita: *Mol. Cryst. Liq. Cryst.* 413, pp. 117-124, 2004.

NVT molecular dynamics simulation is carried out to study the relation of molecular shape and dipole moment to the liquid crystalline ordering at the system of coupled Gay-Berne molecules which are dimers of two types of Gay-Berne particles coupled by harmonic spring at each end. The appearances of polarization and biaxiality together with the location of clearing temperature are reported for various types of combination of position and direction of the dipole attached to molecule.

Ordering in Chiral Smectics at Freely Suspended Film, M. Yamashita: *Ferroelectrics* 309, pp. 63-73, 2004.

The method to study phase transitions of thin systems on the basis of the bulk phase diagram is applied to a freely suspended film of ferroelectric smectics showing a first order phase transition in the bulk, where the ordering effect due to surface layers is replaced by an effective field which is conjugate to the order parameter. In the framework of a phenomenological free energy, whose coefficients are determined from the experimental evidence about C7, behaviours of transition are clarified, which coincides with experimental findings, and especially the small shift of transition temperature from the bulk one is elucidated. The continuous change occurring in the system of thickness just below a critical thickness is proved to be achieved by an insertion of an unstable state of the interior layers, which is never realised in the bulk. This mechanism of continuous change shows the difference between the ordering effects due to the boundaries and external fields.

Isotropic, Nematic and Smectic A Phase Behaviour in a Fictitious Field, M. Torikai and M. Yamashita: *J. Phys. Soc. Jpn.*, 73, pp. 2154-2157, 2004.

Phase behaviours of liquid crystals under external fields, conjugate to the nematic order and smectic order, are studied within the framework of mean field approximation developed by McMillan. It is found that phase diagrams, of temperature vs interaction parameter of smectic A order, show several topologically different types caused by the external fields. The influences of the field conjugate to the smectic A phase, which is fictitious field, are precisely discussed.

Nematic Ordering of a Liquid Crystalline Homeotropic Cell, M. Yasen, M. Torikai and M. Yamashita: J. Phys. Soc. Jpn., 73, pp. 2453-2457, 2004.

Nematic ordering in a very thin system under the homeotropic anchoring condition is studied in the framework of the Maier-Saupe model. Nonuniformity due to the boundary effect is described in terms of an effective field which is conjugate to the order parameter, and behaviour of the system is analysed by observing loci of the effective fields on the phase diagram of the bulk. A continuous change occurring at the system with thickness just smaller than a critical thickness is shown to be mediated by an unstable state; a metastable high-temperature phase changes to a metastable low-temperature one continuously via an unstable phase between them. This mechanism is an analogue of the phenomenon occurring in a freely suspended film of a certain chiral smectic material.

Critical behavior near the metal-insulator transition in the one-dimensional extended Hubbard model at quarter filling, Kazuhiro SANO, Yoshiaki Ono*: Phys. Rev. B70, pp.155102-1-155102-6, 2004.

We examine the critical behavior near the metal-insulator transition (MIT) in the one-dimensional extended Hubbard model with the on-site and the nearest-neighbor interactions U and V at quarter filling using a combined method of the numerical diagonalization and the renormalization group (RG). The Luttinger-liquid parameter (K_F) is calculated with the numerical diagonalization for finite size systems and is substituted into the RG equation as an initial condition to obtain K_F in the infinite size system. This approach also yields the charge gap in the insulating state near the MIT. The results agree very well with the available exact results for $U=\infty$ even in the critical regime of the MIT where the characteristic energy becomes exponentially small and the usual finite size scaling is not applicable.

Antiferromagnetic Exchange Coupling in RE-TM Films, Akira Inagaki, Masaya Tsuneoka, Atsushi Ohshima, Tadashi Kobayashi, Yuji Fujiwara, Shigeru Shiomi and Tsutomu Shiratori*: J. Magn. Soc. Jpn., 28, pp.312-317, 2004.

This paper reports the magnetic and magneto-optical properties of antiferromagnetic exchange coupled (AFC) RE-TM double layered films prepared by sputter deposition. The sample structure is glass/underlayer Ru/Gd-Fe-Co/(E-layer Fe-Co)/AFC layer Ru/(E-layer Fe-Co)/Gd-Fe-Co/protective layer Ru. The exchange coupling energy J was found to depend on Ru thickness of the AFC layer. The first AFC peak was found at an AFC layer thickness of 3.0 Å. Next we inserted a thin Fe-Co layer called the E-layer, between the AFC layer and the magnetic layer to improve the J value. In AFC RE-TM double layered films, a complicated Kerr loop was observed when each magnetic layer was thin. Then we compared the calculated result with the experimental result to distinguish the ferromagnetic coupling from the AFC. Next we investigated thermal stability of J .

Wall Structure and Energy on DWDD, Atsushi Ohshima, Kentaro Kusano, Tadashi Kobayashi, Yuji Fujiwara, Shigeru Shiomi and Masahiko Kaneko*: Trans. Magn. Soc. Jpn., 4, pp.152-155, 2004.

Wall structure and energy have been simulated for the Domain Wall Displacement Detection

(DWDD), and the front process and the rear process under temperature gradient have been considered. For the front process, when the mark length is comparable with the domain wall width in the displacement (D) layer, the domain copied on the D-layer from the memory layer collapses. By making the D-layer thin, the minimum mark length for which the domain wall displacement occurs can be shortened. For the rear process, we confirmed that by inserting the control layer between the D-layer and the switching layer, the mark length with which the ghost signal is suppressed becomes longer. By making the anisotropy energy constant in the D-layer increase, improvement in the DWDD process is expected.

Noncollinear magnetism phenomena induced at surface domain walls and in vortex cores of magnetic quantum dots, A. J. FREEMAN*, Kohji NAKAMURA, Tomonori ITO : *Journal of Magnetism and Magnetic Materials* 272-276, pp. 1122-1127, 2004.

We report noncollinear magnetism phenomena by means of several recent examples: (a) enhancement of magnetocrystalline anisotropy in ferromagnetic (FM) Fe films by intra-atomic noncollinear magnetism, (b) noncollinear magnetic structures of domain walls in FM Fe and antiferromagnetic NiMn, and (c) curling spin and orbital structures in the vortex core of an Fe quantum dot, as obtained from the first principles full-potential linearized augmented plane wave method including noncollinear magnetism with no shape approximation for the magnetization. These results are in good agreement with experiments, and give new information about magnetic phenomena at surfaces and in nanostructures.

Noncollinear magnetism and enhancement of magnetocrystalline anisotropy at the $\Sigma 3(111)$ grain boundary in ferromagnetic Fe, Kohji NAKAMURA, Tomonori ITO, A. J. Freeman*, L. Zhong*, J. F. Castro* : *Applied Physics Letters* 84 , pp. 4974-4976, 2004.

Magnetic structures and magnetocrystalline anisotropy of the $\Sigma 3(111)$ grain boundary (GB) in ferromagnetic Fe are investigated by the first-principles full-potential linearized augmented plane-wave method including intra-atomic noncollinear magnetism. In breaking the spatial translation symmetry in a crystalline solid, GB is found to give rise to a magnetic noncollinearity, where the magnetic moments at both sides of the GB orient at an angle about 10° with respect to each other. Importantly, the presence of the GB enhances the magnetocrystalline anisotropy energy by one order of magnitude from its bulk value and may induce a pinning effect on the magnetization rotation or magnetic domain wall motion.

Atomically sharp magnetic domain wall in thin films Fe(110): A first principles noncollinear magnetism study, Kohji NAKAMURA, Yoshifumi TAKEDA, Toru AKIYAMA, Tomonori ITO, A. J. Freeman* : *Physical Review Letters* 93, pp.057202-1-4, 2004.

Magnetic domain wall structures in an Fe(110) monolayer are determined by the highly precise first principles full-potential linearized augmented plane-wave method including intra-atomic noncollinear magnetism. The self-consistent results demonstrate that the magnetization changes from one orientation to the opposite (180°) orientation within 8 Å width without any abrupt rotation. This

narrow domain wall is found to arise from band effects. Our results are consistent with and support domain walls having a 6 Å width recently observed in spin-polarized scanning tunneling microscopy experiments.

Magnetic structures and out-of-plane magnetic anisotropy at the exchange bias interface: Co/FeMn, Kohji NAKAMURA, Tomonori ITO, A. J. Freeman* : *Physical Review B* 70, pp. 060404(R)-1-4, 2004.

The magnetic structures and anisotropy at the compensated ferromagnetic/antiferromagnetic Co/FeMn interface are investigated by the highly precise first principles full-potential linearized augmented plane-wave method that incorporates intra-atomic noncollinear magnetism in order to understand the magnetic complexity involved in the spin-flop coupling and the presence of intra-atomic noncollinear magnetism. The self-consistent results predict that the Fe moments in the FeMn layer reorient away from their directions in bulk FeMn so as to be parallel to the Co moment direction – a reorientation that induces an out-of-plane magnetic anisotropy. These results appear to support and confirm recent experimental x-ray magnetic circular dichroism findings that rule out spin-flop coupling as the mechanism for exchange bias in this system.

Modern computational magnetism: role of noncollinear magnetism in complex magnetic phenomena, A. J. FREEMAN* and Kohji NAKAMURA: *Physica Status Solidi (b)* 241, pp. 1399-1405, 2004.

Modern computational magnetism continues to grow at an accelerating pace stimulated by new and exciting discoveries important for basic science and technological applications. Here, we review some recent important progress made in treating complex noncollinear magnetic phenomena arising from the breaking of symmetry at surfaces, interfaces, and nanostructures, by means of our newly generalized first principles full-potential linearized augmented plane wave (FLAPW) method for noncollinear magnetism with no shape approximation to the magnetization. Because of space limitations, we restrict our report illustrate results of the noncollinear magnetic structures induced at the FM NiFe/AFM NiMn interfaces, in the domain walls of FM Fe and AFM NiMn, and in the vortex cores of a Fe quantum dot. These results are in good agreement with experiments and give new information about magnetic phenomena at surface, interfaces, and in nanostructures.

Systematic theoretical investigations of adsorption behavior on the GaAs(001)-c(4x4) surfaces, Tomonori ITO, Kazumi TSUTSUMIDA, Kohji NAKAMURA, Yoshihiro KANGAWA*, Kenji SHITRAISHI*, Akihito TAGUCHI*, Hiroyuki KAGESHIMA* : *Applied Surface Science* 237, pp. 194-199, 2004.

Adsorption behavior on the GaAs(001)-c(4x4) surfaces is systematically investigated by using our ab initio-based approach and the Monte Carlo methods. The change in stable structure of the c(4x4) surfaces is clarified by considering adsorption or desorption of surface dimers as functions of temperature and As pressure. The calculated results imply that the c(4x4) surface with As dimers is stable at low temperatures less than ~400 K, whereas the surface with Ga-As dimers is stabilized at high temperatures in the range of ~400 K to ~700 K. The disordered dimer arrangements consisting of Ga and As substituted by each other in the c(4x4) unit cell hardly appear even at high temperatures

such as ~800 K. We also investigate the behavior of Ga and As adatoms on these $c(4 \times 4)$ surfaces. The calculated results reveal that Ga atoms can adsorb and migrate on the surfaces while desorption of As adatoms proceeds without sufficient migration.

Theoretical investigations of adatom behavior on non-planar surfaces with GaAs($n11$)A, Koichi ASANO, Yoshihiro KANGAWA*, Hirotoishi ISHIZAKI, Toru AKIYAMA, Kohji NAKAMURA, Tomonori ITO : *Applied Surface Science* 237, pp. 206-212, 2004.

The behavior of Ga and As adatoms on non-planar surfaces consisting of GaAs(001)-(2x4) and GaAs($n11$)A ($n=2, 3$ and 4) surfaces are investigated by empirical interatomic potentials with the aid of ab initio calculations. The calculated results imply that Ga adsorption energies strongly depend on the surface orientation, whereas As adsorption energies keep almost constant. The difference in adsorption energies can be interpreted by considering strain energy. In particular, Ga adatom is stabilized on the (311)A surface by the smallest strain energy forming interatomic bonds with three As atoms located at the regular fcc sublattice. Furthermore, we roughly simulate resultant surface profile of GaAs thin films on the non-planar surfaces consisting of the (001)-(2x4) top and ($n11$)A side surfaces based on the rate equation. The simulated results reveal that the non-planar surface with (311)A side surface forms the linear surface profile.

First-principles analyses of O₂ molecules around ultrathin SiO₂/Si(100) interface, Toru AKIYAMA, Hiroyuki KAGESHIMA*, Tomonori ITO : *Japanese Journal of Applied Physics* 43, pp. 7903-7908, 2004.

The microscopic structures and reaction mechanisms of O₂ molecules at ultrathin SiO₂/Si(100) interface are investigated based on first-principles total-energy calculations. It is found that the molecular-type oxygen is stable in the SiO₂ region of the interface, while the O₂ in the Si substrate dissociates and two Si-O-Si bonds are formed. It is also found that the O₂ in the SiO₂ region can directly react with the Si substrate. The energy barrier for its reaction (0.2 eV) does not correspond to (previously consented) serving process of interfacial Si-Si bonds, but to the formation of weak Si-O bonds between the O atoms of oxidant and the interfacial Si atoms: The hybridization of the oxygen-2p orbitals of the oxidant and the valence band states of the Si substrate is the principal factor of the reaction. The calculated results imply that other microscopic mechanisms such as accumulation of interfacial strain or its release mechanisms are involved in the interfacial reaction during Si oxidation.

Theoretical study of excess Si emitted from Si-oxide/Si interface, Hiroyuki KAGESHIMA*, Masashi UEMATSU*, Kazuto AKAGI*, Shinji TSUNUYUKI*, Toru AKIYAMA, Kenji SHIRAISHI* : *Japanese Journal of Applied Physics* 43, pp. 8223-8226, 2004.

The excess Si emitted from the Si-oxide/Si interface is studied using the first-principles calculations. It is shown that the excess Si can have many (meta-) stable positions around the interface. In addition, some positions in the oxide do not have any dangling bonds or floating bonds in contrast to those in the bulk crystalline Si. The results indicate that the emitted Si can be located in the oxide layer

but they do not necessarily cause charge traps in the oxide. The emitted Si atoms are thought to just be oxidized and absorbed into the oxide while a portion of them cause the E' centers, the P_b centers or charge traps.

Thermodynamic stability for group IV alloy semiconductors [in Japanese]. Tomonori ITO, Yoshihiro KANGAWA* : Journal of the Japanese Association for Crystal Growth 31, pp. 4-11, 2004.

Thermodynamic stability of group IV alloy semiconductors such as $\text{Si}_{1-x}\text{Ge}_x\text{C}_y$ solid solutions in bulk and thin film states is systematically investigated by excess energy calculations based on empirical interatomic potentials and Monte Carlo (MC) simulations. In bulk state, the calculated excess energies for $\text{Si}_{1-x}\text{Ge}_x\text{C}_y$ have positive values over the entire concentration range. This implies that $\text{Si}_{1-x}\text{Ge}_x\text{C}_y$ with a random distribution of Si, Ge and C is thermodynamically unstable at 0 K. Furthermore, the excess energies of $\text{Si}_{1-x}\text{Ge}_x\text{C}_y$ increase with Ge content x when C content y remains constant. This is because an increase of Ge content introduces large strain energy in $\text{Si}_{1-x}\text{Ge}_x\text{C}_y$. In thin film state, although lattice constraint at the interface reduces the excess energies by 20-30 % of those in bulk state, we obtain similar results to those in bulk state. Further MC simulation reveal that Ge atoms segregate in the topmost layer and C atoms accumulate in the second layer.

Plastic Deformations of Micro-Spheres by Solidified Lubricants and Lubricants' Shear Characteristics under Very High Pressure (Part 1) - Observation of Plastically-Deformed Micro-Spheres - [in Japanese], Yuichi NAKAMURA, Yutaka ISHIBASHI* and Yasushi KUROSAKI: Tribologist, 49-6, pp. 518-524, 2004.

Fractal analysis of adhesion on tool surface in compression of aluminum strips by using AFM [in Japanese], Masahito MATSUI, Yasushi KUROSAKI and Yusuke MIYAUCHI: Journal of Japan Institute of Light Metals, 54-1, pp. 9-13, 2004.

Adhesion properties in simple compression of aluminum strips are analyzed in the micro/nanometer range by employing the zero set and power spectrum fractal analyses. An atomic force microscope (AFM) is used to estimate the fractal dimensions. It is found that the adhesion and tool and specimen surfaces have fractal structure. Various fractal dimensions obtained for the adhesion and tool and specimen surfaces are compared to each other and discussed. When the surface roughness of tool is same, the ratio of the total adhesion area depends on the fractal dimension. Though the AFM apparatus is difficult to distinguish the adhesion particles from the tool surface, the power spectrum dimension has possibility of distinguishing the adhesion particles from the tool surface. Finally, a method for computer simulation of the nanometer scale surface structure is presented, and satisfactory images are constructed.

Nanofractal Analysis on Material Surfaces Using AFM, Mir Behdad Khamesee, Yasushi Kurosaki, Masahito Matsui and Kenichi Murai: Materials Transactions, 45-2, pp. 469-478, 2004.

The surface structures of four materials (a pure aluminum sheet, an aluminum alloy sash, a

thickness gauge and a magnetic tape) are observed on the nanometer scale by atomic force microscopy (AFM) and analyzed by one-dimensional fractal analyses. It is confirmed for all the surfaces that they have a self-affined fractal property under a resolution of 1nm. The two-dimensional fast Fourier transformation (2D-FFT) analysis is also applied to these surfaces and their characteristics are clarified. The power spectrum model for surface simulation is proposed and its validity is confirmed by experimental results. A method for simulating surface structure of any materials is presented, and its validity is shown on some materials whether in-plane isotropic or anisotropic. A computer aided engineering (CAE) system composed of 2D-FFT and inverse FFT (IFFT) for quantitative estimation of surface nanostructures is advanced and applied to various surface problems. It enables the mass data of material surface to compress into only three parameters.