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Successive Phase Transitions in Antiferroelectric Liquid Crystal Systems -An Axial Next-Nearest-Neighbor XY Model with Biquadratic Interaction, M. Koroishi, M. Torikai and M. Yamashita: Ferroelectrics 344, 125-132, 2006

An axial next-nearest-neighbor XY model is studied as a model of chiral liquid crystals which exhibit many ferro-, ferri- and antiferroelectric tilted smectic phases. Depending on the values of interaction parameters, this model exhibits Ising symmetric (i.e., the tilt directions of directors are parallel or anti parallel) phases or XY symmetric phases. Phases with each type-of-symmetry show the character of devil's staircase, which has been observed in experiments.

Symmetry of Nematic Phase and Oblique Axial Order, M. Yamashita and M. Torikai: J. Phys. Soc. Jpn., 75, 104601-1-6, 2006

Nematic order is usually described by a uniaxial order parameter, or occasionally by a biaxial order parameter together with the uniaxial one, in a typical configuration. In a general case of a system exposed to two different types of external fields, e.g., an electric field and a magnetic field, an additional order parameter, here called an oblique axial order parameter, is shown to be necessary, in addition to the above order parameters, to describe transition phenomena of the system correctly. The symmetry of the phase with the triplet of the order parameters is discussed. Effect of the oblique axial order are demonstrated practically in two phenomena: (i) qualitative change of the phase transition when the oblique axial order is neglected; (ii) disappearance of phase transition between ordered phases with different ordering axes when an oblique axial field conjugate to the oblique axial order parameter exists.

Nematic and Smectic Orderings and Commensurability at Thin Liquid Crystal System, S. Murayama, S. Taira, M. Torikai, T. Miyazaki and M. Yamashita: Proceedings of the 13th Tri-University International Joint Seminar & Symposium 2006, 364-367, 2006

Liquid crystalline ordering at a very thin system is simulated to study an effect of boundary walls, especially, due to a thickness of the system. The system is composed of Gay-Berne particles of standard values of force parameters, which is sandwiched by parallel walls of homeotropic anchoring. Molecular dynamics simulation is carried out at an NVT ensemble. The system exhibits isotropic, nematic and smectic phases successively as a temperature is decreased. The transition temperature between the nematic phase and the smectic one is shown to change oscillatory as the thickness of the system is increased, and this phenomenon is interpreted as an outcome of a commensurability of the thickness to a layer spacing of the smectic structure.

An empirical potential approach to wurtzite-zinc blende polytypism in group III-V semiconductor nanowires, Toru AKIYAMA, Kosuke SANO, Kohji NAKAMUARA, Tomonori ITO: Japanese Journal of Applied Physics, 45, pp.L275-L278, 2006.

The relative stability between wurtzite and zinc blende structures in group III–V semiconductor nanowires is systematically investigated based on an empirical potential, which incorporates electrostatic energy due to

valence-bond and ionic charges. The energy differences between wurtzite and zinc blende structures of 12 compound nanowires with diameter of 1–22 nm show that the wurtzite nanowires are stabilized for small diameter. This structural trend is found to be due to the contribution of two- and three-coordinated atoms on the nanowire facets to the system energy. We also find that the critical diameters, where the nanowires turn out be bistable forming both wurtzite and zinc blende structures, exist at the diameter of 12–32 nm depending on the ionicity of semiconductors. The bistability implies the synthesis of nanowires exhibiting polytypes, and supports the experimental results in GaP, GaAs, InP, and InAs nanowires.

Mechanism of oxide deformation during silicon thermal oxidation, Hiroyuki KAGESHIMA*, Masashi UEMATSU*, K. AKAGI*, Shinji TSUNEYUKI*, Toru AKIYAMA, Kenji SHIRAISHI*: Physica B, 376-377, pp.407-410 , 2006.

Mechanisms of oxide deformation during silicon thermal oxidation are studied by investigating the energetics of intrinsic point defects in the bulk silicon oxide and in the oxide film of the silicon oxide/silicon interface with first-principles calculations. The results suggest that the SiO_2 and the SiO interstitials are thought to relate to the deformation of the silicon oxide. Especially, during the silicon oxidation, the SiO interstitial is suggested to be important because it can be formed in the oxide film neighboring to the interface and can enhance the deformation of the oxide films.

A simple approach to polytypes of SiC and its application to nanowires, Tomonori ITO, Kosuke SANO, Toru AKIYAMA, Kohji NAKAMURA: Thin Solid Films, 508 , pp.243-246, 2006.

SiC polytypes in bulk form and nanowire are systematically investigated using our empirical potential that is based on a simple approach, and which incorporates electrostatic energies due to bond charges and ionic charges. Using the empirical potential, the system energies of 3C (zinc blende), 6H, 4H and 2H (wurtzite) structured SiC in bulk form are calculated and compared with ab initio calculations and experimental results. Our calculated results reveal that 3C–SiC is the most stable while 2H–SiC is unstable among these structures at 0 K. This is consistent with experimental results. The appearance of polytypes in bulk form is qualitatively discussed by considering ionicity of semiconductors based on our simple approach. Furthermore, we clarify the versatility of our simple approach to nanostructures considering SiC nanowire. Hexagonal SiC nanowire stabilizes a 2H structure in the diameter range of $D < 20$ (nm), whereas 3C–SiC is stabilized only at a large diameter range beyond 20 (nm). This is also consistent with experimental findings for InAs and InP nanowires. SiC polytypes in nanowire are discussed in terms of the ratio of the number of surface dangling bonds to the total number of interatomic bonds.

A first-principles study of O_2 incorporation and its diffusion in compressively strained high-density silicon oxides, Toru AKIYAMA, Keiichi KAWAMOTO, H. KAGESHIMA*, M. UEMATSU, Kohji NAKAMURA, Tomonori ITO: Thin Solid Films, 508, pp.311-314, 2006.

The microscopic mechanisms of O_2 diffusion in compressively strained high-density silicon oxides are investigated based on first-principles total-energy calculations. It is found that, both in high-density α-quartz and in α-cristobalite, the calculated incorporation energies and energy barriers increase with increase of oxide density. Independent of the structure of oxides, the calculated activation energies increase with increasing density. Furthermore, the calculated activation volumes suggest that the oxidation retardation by the oxidation-induced strain is due to the retardation of O_2 diffusion in the high-density region, qualitatively consistent with experimental results.

Spin-spiral structures in free-standing Fe(110) monolayers, Kohji NAKAMURA, Naoki MIZUNO, Toru AKIYAMA, Tomonori ITO, A. J. FREEMAN*: Journal of Applied Physics, 99, pp.08N501-1-3, 2006.

Electronic and magnetic structures in spin-spiral structures of free-standing Fe(110) monolayers with lattice constants, a, matching those of bulk bcc Fe (2.87 Å) and W (3.16 Å), were investigated by means of first-principles film full-potential linearized augmented-plane-wave calculations including intra-atomic noncollinear magnetism. For a=2.87 Å, the spin-spiral structures with wavelength around 7a are energetically favored over the collinear ferromagnetic state while those for a=3.16 Å turn out to be less favorable. The formation of the spin-spiral structures are found to result from a Fermi-surface nesting that leads to an instability of the ferromagnetic state. In addition, the spin-orbit coupling is found to play an important role to determine the magnetization rotation. These results offer an important step in understanding complex noncollinear spin-spiral magnetism in thin films.

Structural stability and electronic structures of InP nanowires: Role of surface dangling bonds on nanowire facets, Toru AKIYAMA, Kohji NAKAMUR, Tomonori ITO: Physical Review B, 73, pp.235308-1-6, 2006.

The structural stability and electronic properties of InP nanowires (NWs) are investigated based on first-principles pseudopotential calculations. In contrast to the bulk phase, zinc-blende (ZB) NWs are found to be less favorable over wurtzite (WZ) NWs, in which the surface dangling bonds (DBs) on the NW facets play a crucial role to stabilize the WZ structure. Our analysis of the NW cohesive energy based on the number of DBs also suggests the bistability forming both ZB and WZ NWs around 120 Å diameter and the formation of rotational twin structures around 400 Å diameter being consistent with experiments. Furthermore, the stable WZ NWs are found to be semiconducting whose characteristics are dependent on the surface DBs as well as the NW size and shape. The estimated oscillator strength also indicates the possibility of efficient light emission originating from the direct gap and geometrically restricted excitonic effects.

Stacking sequence preference of pristine and hydrogen-terminated Si nanowires on Si(111) substrates, Toru AKIYAMA, Kohji NAKAMURA, Tomonori ITO: Physical Review B, 74 , pp.033307-1-4, 2006.

The hexagonal versus cubic structural preference in vertically grown silicon nanowires on Si(111) substrates is systemized by using first-principles pseudopotential calculations. The calculated formation energy for pristine and H-terminated silicon nanowires with both hexagonal and cubic stacking sequences demonstrates that the stability depends on hydrogen chemical potential and the hexagonal-type nanowires are energetically favorable over a wide range of hydrogen chemical potential. This preference offers a possible origin for little detection of the [111]-oriented silicon nanowires with small diameters, qualitatively consistent with experimental findings.

Thermodynamic stability of $In_{1-x-y}Ga_xAl_yN$ on GaN and InN, Yoshihiro KANGAWA*, Koichi KAKIMOTO*, Tomonori ITO, Akinori KOUKITSU*: Physica Status Solidi (c), 3, pp.1700-1704, 2006.

Monte Carlo simulations of InGaN MOVPE were carried out to investigate the relationship between growth conditions and atomic arrangement in thin films grown on (0001) and (11 0). In the case of small input partial pressures of indium, it was found that compositional instability was enhanced during the site exchanging process

instead of the adsorption process. Moreover, it was found that compositional fluctuation in thin films grown on (11 0) is smaller than that in thin films grown on (0001). This suggests that accumulated stress near the growth surface influences the compositional fluctuation.

Theoretical study on atomic structures of thermally grown silicon oxide/silicon interfaces, Hiroyuki KAGESHIMA*, Masashi UEMATSU*, K. AKAGI*, Shinji TSUNEYUKI*, Toru AKIYAMA, Kenji SHIRAISHI*: e-Journal of Surface Science and Nanotechnology, 4, pp.584-587, 2006.

The reason why previous researchers have repoterd many different atomic structures such as cristobalite, tridymite, and quartz for the thermally grown silicon oxide/silicon interfaces is studied by following the possible interface structures during the oxidation processes using the first-principles calculations. The results show that the cristobalite-like structures can be easily formed from the silicon diamond structure. Proceeding with the oxidation, compressive strains are accumulated in these cristobalite-like regions. To significantly release these accumulated strains, it is considered that the cristobalite-like regions change into less strained tridymite-like structures and finally more relaxed quartz-like structures. If the transformation occurs without lateral ordering, then the transformed interfacial structure does not have any order and should be amorphous. This explanation provides us with a unified understanding of the interfacial atomic structures.

Oxygen trap hypothesis in silicon oxide, Hiroyuki KAGESHIMA*, Masashi UEMATSU*, Toru AKIYAMA, Tomonori ITO: Japanese Journal of Applied Physics, 45, pp.7672-7674, 2006.

A hypothesis on the atomic structure of silicon oxide is proposed to explain the discrepancy between theoretical and experimental studies on the oxygen diffusion and the interfacial reaction during the thermal silicon oxidation process. The hypothesis says that silicon oxide contains "oxygen traps", in which the molecular oxygen can be located with almost 0 dissolving enthalpy. The density of the "traps" is ~10^{16} cm^{-3}. A possible local structure is also proposed based on the first-principles calculations.

Magnetic and electronic structures of zinc-blende ferromagnetic/antiferromagnetic Interfaces, Yoshinori KATO, Toru AKIYAMA, Kohji NAKAMURA, Tomonori ITO: e-Journal of Surface Science and Nanotechnology, 4, pp. 58-62, 2006.

Magnetic structures at zinc-blende ferromagnetic (FM) and antiferromagnetic (AFM) interfaces, CrAs/Cr, CrAs/GaAs/Cr, and CrSe/MnSe, were investigated by means of the full-potential linearized augmented plane-wave method in order to search the half-metallic exchange bias interfaces. The CrAs/Cr structure is found to lose the half-metallicity at the CrAs interface while the CrAs/GaAs/Cr structure retains the half-metallicity but the energy difference between parallel and antiparallel moment alignments of the FM and AFM layer at the interface significantly reduces. In contrast, the CrSe/MnSe interface induces an excellent half-metallicity, which importantly offers a key ingredient as a promising half-metallic exchange bias.

Half-metallic exchange bias ferromagnetic/antiferromagnetic interfaces in transition-metal chalcogenides Kohji NAKAMURA, Yoshinori KATO, Toru AKIYAMA, Tomonori ITO, A. J. FREEMAN: Physical Review Letters, 96, (4), pp. 047206-1-4, 2006.

To investigate half-metallic exchange bias interfaces, magnetic structures at ferromagnetic (FM)/antiferromagnetic (AFM) interfaces in the zinc blende transition-metal chalcogenides, CrSe/MnSe and CrTe/MnTe with compensated and uncompensated AFM interfaces, were determined by the full-potential linearized augmented plane-wave method. With the uncompensated AFM interface, an antiparallel alignment of the Cr and Mn moments induces an excellent half-metallicity. More striking still, in the compensated AFM interface the Cr moments in the FM layer lie perpendicular to the Mn moments in the AFM layer but the Mn moments strongly cant to induce a net moment so as to retain the half-metallicity. These findings may offer a key ingredient for exchange biased spintronic devices with 100% spin polarization, having a unidirectional anisotropy to control and manipulate spins at the nanoscale.

Transport mechanism of interfacial network forming atoms during silicon oxidation, Hiroyuki KAGESHIMA*, Masashi UEMATSU*, K. AKAGI*, Shinji TSUNEYUKI*, Toru AKIYAMA, Kenji SHIRAISHI*: Japanese Journal of Applied Physics, 45, pp. 694-699, 2006.

A first-principles study on the energetics of the structural transformation at the interfaces revealed that oxygen vacancies can accompany the high density oxide regions formed during the silicon oxidation. The vacancies can also promote the effective out-migration of these regions, which allows the easier oxide viscous flow to release the interfacial strain. Compared with this mechanism, self-interstitials are rarely formed in the silicon substrate. These results also suggest defect formation mechanisms around the interfaces.

Development of a Super Broadband RF Splitter Using Bead Type Ferrite Core Transformers, T. KANIE*, H. KATO, Y. NORO and T. TAKEO: Proc. of 11th International Ceramic Congress Advances in Science and Technology 45, pp.2576-2581, 2006

Recent developments in information technologies require various communication devices to operate at a higher speed and in a wider frequency range in order to accommodate a vast amount of data. A RF Splitter whose function is to divide an input signal into multiple outputs is the most popular passive device in CATV networks and consists of transformers using ferromagnetic materials such as ferrite. Nowadays, because of the circumstances stated above, the RF splitter for CATV systems must operate in an extremely wide frequency range in order to transmit a large number of channels multiplexed with a frequency division technique. In other words, its loss should be as small as possible in that region. We have studied the broadening of the operative frequency by investigating how the ferrite core parameters including the magnetic permeability, shape, surface mounting of the core, etc. affect the transmission characteristics. We examined the relationship between each of these parameters and the transmission characteristics through a computer simulation and fabricated a device based on the calculations. It was found that by selecting the appropriate parameters, excessive splitter loss could be suppressed to less than 3.5dB in the range of 10MHz to 3,000MHz.

Preparation of Magnetic Tunnel Transistors with Double Tunnel Junctions, Haruki NAKANISHI, Haruki OMAE, Yuji FUJIWARA, Mutsuko JIMBO*, Tadashi KOBAYASHI, Shigeru SHIOMI: J. Magn. Soc. Jpn., 30, pp.188-191, 2006.

Magnetic tunnel transistors (MTTs) with double tunnel junctions were prepared in order to investigate the emitter voltage dependence of a magneto-current (MC). A three-terminal structure was fabricated, using metal shadow masks. It was observed that hot

electrons contributed to a collector current. A transfer ratio of over 10^{-3} was obtained in an MTT with double tunnel junctions. The MC decreased gradually with increasing emitter voltage. The emitter voltage at which the MC decreased to half its original value was over 1.5 V.

Magnetics Education in Companies, Magnetics Education in Universities, Tadashi KOBAYASHI: Magn. Jpn., 1, pp.370-374, 2006.

It seems that some gap exists between magnetics education in companies and in universities. To bridge the gap, if necessary, universities should deliver lectures to companies. Furthermore, universities should educate students to obtain an exact understanding of physical phenomena. For this purpose, experience is very important. Various teaching materials for experiments are introduced, e.g. diamagnetic substances and magnets to demonstrate repulsion, paramagnetic substances and magnets to demonstrate attraction, speakers made from corrugated boxes, and microphones. It is also important to show that how theory is put to practical use.

Oil Solidified High-Pressure Traction Curve Estimation with Spin by Elastic Contact Mechanics, Yuichi NAKAMURA and Masane FUNAHASHI: Trans. of JSME, Ser. C, 72-717, pp. 1653-1659, 2006

Traction curves are fundamental data for the design of traction-type continuously variable transmission (tCVT) of automobiles, in which maximum hertzian contact pressure exceeds 3GPa. Under such high contact pressure, oils seems to behave like solid lubricants and elastic contact mechanics (creep theory) seems to be appropriate for evaluation of traction curves similar to that of railway wheels. In the present study, oil-solidified high-pressure traction curves with spin were roughly and simply calculated up to 3 GPa based on creep theory together with maximum traction coefficients of pure roll experimental data of reference. Calculated curves were almost consistent with several reference experimental ones of various conditions (speed, geometry of test machine). This consistency proved that main factor of oil-solidified high-pressure traction curves with spin is creep theory and main rheological property of oils is the limiting shear stress.

High-Pressure Viscosity Measurements of Vegetable Based Biodegradable Lubricant Oils up to 2.5 GPa and Tribological Characteristics, Y. Nakamura, H. Matsubo, K. Yoshizaki and H. Komiya,: Proc. Int. Tribology Conf., Austrib 2006, CD, 108, pp. 1-6, 2006

In order to provide environmentally friendly lubrication with high-pressure rheological and tribological data of several biodegradable vegetable oils, their viscosity and phase transition were evaluated up to 2.5 GPa at up to 200℃ employing a falling sphere method in a diamond-anvil pressure cell. Also, friction and wear properties for these oils were evaluated employing a SRV tribo-tester. Similar high-pressure viscosity characteristics of 7 oils including rapeseed oil, soybean oil and polyol ester (POE) were observed. The pressure-viscosity coefficients of all the oils around the maximum pressure were 12 /GPa at 0.2-0.4 GPa and at 40℃, 7 /GPa at 0.5-1.4 GPa and at 100 ℃, 3-4 /GPa at 1.8-2.7 GPa and at 200℃. For most oils, the sphere stopped falling over about 10 Pa･s at all temperatures and pressures evaluated. Finally, lubricant oils, except POE, were observed to transit to polycrystal-like phase. Friction coefficients for the vegetable oils were evaluated between 0.09 and 0.12, and between 0.12 and 0.14 for POE. The wear amount of POE was observed to be more than twice larger than that of the vegetable oils.

Fabrication of LSMO Single Layers and LSMO/YBCO Double Layers, Hong ZHU, Masanori OKADA, Atsushi KAMIYA, Ajay Krishno SARKAR, Masahito MATSUI, Md. Motin SEIKH and Tamio ENDO: International Journal of Nanoscience, 5– 4 & 5, pp. 511–515, 2006

(La, Sr)MnO3 (LSMO) single-layer and LSMO/YBCO double-layer films have been grown on LAO and MgO substrates using ion beam sputtering. For LSMO single-layer films, the highly epitaxial films can be grown at lower substrate temperatures down to 500ºC. The epitaxy of the films, which is degraded with increasing TS, can be restored by supply of plasma oxygen. Smaller lattice mismatch of LSMO on LAO gives two-dimensional step-and-terrace type growth, whereas on MgO grain type growth is observed due to larger mismatch. For the double-layer films, LSMO layer can be grown epitaxially on a-oriented YBCO underlayer, but a part of the underlying a-YBCO is changed into c-YBCO during the deposition of overlayer. For c-YBCO underlayer, a part of the underlying c-YBCO is changed into (110)-oriented phase after the deposition of overlayer. Then it is necessary to deposit the overlayer at lower temperatures.