

## Nanomaterials

Room: Mauka - Session NM-TuP

### Nanomaterials Poster Session

**NM-TuP1 Electronic Structure of Titanate Nanoribbons Studied by O 1s and Ti 2p X-Ray Absorption and 3-Dimensional Dichroism Measured in a Scanning Transmission X-ray Microscope (STXM), Adam Hitchcock, X. Zhu, McMaster University, Canada, C. Bittencourt, University of Mons, Belgium, P. Umek, Jožef Stefan Institute, Slovenia, P. Krüger, Chiba University, Japan**

TiO<sub>x</sub>-based nanostructures are being used as active materials in lithium ion batteries, gas sensors, photocatalysts, dye synthesized solar cells, etc. Much effort has been directed toward understanding their electronic properties [1] because they exhibit physical and chemical properties different from their bulk counterparts. They are challenging to study by analytical electron microscopy techniques since they are highly sensitive to radiation damage. Their nano-scale prevents the use of conventional X-ray absorption spectroscopy (NEXAFS) to study individual structures. Scanning transmission x-ray microscopy (STXM) allows studies of the electronic structure of individual nanomaterials with high spatial resolution (30 nm) and high energy resolution (0.1 eV) via NEXAFS spectroscopy and its linear dichroism (spectral variation as a function of the E-vector orientation) [2]. Here we report STXM-NEXAFS studies of individual sodium titanate nanoribbons (NaTiO<sub>x</sub>-NR) prepared by hydrothermal treatment of anatase TiO<sub>2</sub> micro-particles [3]. By measuring the dichroism with the sample at different orientations relative to the X-ray beam, and varying the direction of the linear E-vector by an elliptically polarizing undulator (EPU), the linear dichroism at the O 1s and Ti 2p edges was measured along the 3 principle axes of the anisotropic nanoribbons. Comparison of the spectra and dichroism with high level calculations helps confirm the crystal structure [4] and gives insight into the electronic bonding in these novel layered materials through the orientation dependence of local electronic structure within the crystallite. The methodology for 3D dichroic STXM measurements newly developed in this study is a powerful way to investigate anisotropic nanomaterials.

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**NM-TuP3 VOC Degradation Ability of VO<sub>x</sub>-TiO<sub>2</sub> Mixed Nanoparticles Attached on Glass Fiber in the Flow Chamber Test, Seonmin Kim, KETI, Republic of Korea, Baron. Cho, KETI**

VO<sub>x</sub>-TiO<sub>2</sub> nanocomposite samples made by one-pot synthesis showed the various catalytic activities depending on the calcination temperature. Photocatalytic activity of VO<sub>x</sub>-TiO<sub>2</sub> nanoparticles fabricated at various temperatures were characterized by the degradation of methylene blue in aqueous solutions under UV irradiation. Nanocomposites show significant enhancement of decomposition of methylene blue and the reason is considered by the synergistic effect between two different materials. In this study, the prepared nanocomposite catalysts were attached on glass fiber by cross-linking method and photodegradation abilities were tested by the change of VOC gas concentration in a closed chamber. For the photocatalytic analysis of the prepared nanoparticles, the absorption spectra are measured by UV-visible spectrophotometer and the bandgap analysis are performed by Kubelka-Munk theory. VOC removal abilities are quantified by the variation of p-xylene concentration in the closed chamber. Obtained results show that the as-prepared VO<sub>x</sub>-TiO<sub>2</sub> nanocomposites have different degradation abilities depending on the calcination temperature and vanadium atomic percentage.

**NM-TuP4 Surface Modification of TiO<sub>2</sub> Nanoparticles with Organic Molecule and Their Selective Adsorption Activity Toward Proteins, Xia Zhang, Northeastern University, China**

The nanomaterials have been widely applied in the biomedical area, which play important role in the disease diagnosis and treatment, tissue repair and proteins separation. Nano-TiO<sub>2</sub>, as a biologically inert material, shows good biocompatibility and bonding biological activity of the protein. In addition,

the surface modification of TiO<sub>2</sub> can be achieved by the surface bonding between its surface hydroxyl groups and organic molecules. Furthermore, the research on the selective adsorption of proteins on the functionalized nanomaterials has important theoretical significance and application value in the field of protein separation.

In this work, TiO<sub>2</sub> nanoparticles were prepared by improved hydrothermal method, and then some organic molecule, such as silane KH560 and oleic acid were used to modify the TiO<sub>2</sub> nanoparticles. Some means, such as TEM, XRD, TG-DSC, and FT-IR were used to character the functionalized TiO<sub>2</sub> nanoparticles. The results showed that the organic molecules were successfully combined on the surface of TiO<sub>2</sub> nanoparticles via chemical bond and physical weak interaction.

These functionalized TiO<sub>2</sub> nanoparticles were used in the adsorption experiments of bovine hemoglobin (Bhb) and bovine serum albumin (BSA). The effects of different conditions on the adsorption capacity were studied systematically, and the optimum adsorption conditions were determined. Compared with the original nano-TiO<sub>2</sub>, after surface modification, the functionalized TiO<sub>2</sub> nanoparticles showed selective adsorption activity toward Bhb. For example, under optimum conditions (*c*<sub>0</sub> (Bhb or BSA) = 150 mg/L, *m* (TiO<sub>2</sub>) = 0.8 mg/mL, *t* = 80 min.), for the pure TiO<sub>2</sub> nanoparticles, the adsorption capacity of Bhb and BSA was 70.6 mg/g and 40 mg/g respectively. Meanwhile, for the KH560 modified TiO<sub>2</sub>, the maximum adsorption capacity of Bhb was 122.8 mg/g and the adsorption of BSA was almost 0.

**NM-TuP5 Spontaneous Oxidation and Exfoliation of Graphene Oxide using Couette-Taylor Reactor, W.K. Park, Hyongkeun Kim, Korea Electronics Technology Institute, W.S. Yang, Korea Electronics Technology Institute, Republic of Korea**

For the application of reduced graphene oxide to industries, an eco-friendly reduction method and shortening of the pickling and oxidation reaction times in the graphene oxide production process are essential. We dramatically shortened the graphene oxide production time by applying the Couette-Taylor flow, which allows consecutive reactions, to the graphite oxidation process using the modified Hummers method. With a 60-minute oxidation reaction in the Couette-Taylor reactor, the interlayer spacing increased from 0.34 nm to 0.78 nm, and uniform single- to multi-layer graphene oxides were obtained at a high yield of 93%. The properties of fabricated GO was examined by field emission scanning electron microscope, Raman spectra, atomic force microscope, x-ray photoelectron spectroscopy and x-ray diffraction.

**NM-TuP6 Field Emission and Anomalous Light Emission from Isolated ZnO Nanorods Array under Lateral Electric Field Application, T. Hirate, Kanagawa University, Japan, Yu Miura, T. Satoh, Kanagawa University**

We study on electrical and luminescent characteristics of ZnO nanorods array when an electric field is applied in lateral direction to the axis of ZnO nanorods.

ZnO nanorods are grown by chemical vapor deposition after laser ablation of gold on substrate. This growth method was developed by us. Glass substrates (26 mm x 26 mm) are coated with SiO<sub>2</sub> film of 100 nm thickness by electron-beam deposition. The length of ZnO nanorods is about 1 micron meter and the diameter is from 50 nm to 80 nm. The direction of nanorods is distributed around a vertical axis to substrate surface.

The mean separation between nanorods on the area between electrodes is about 1.5 micron meter, and nanorods are isolated with each other. This is confirmed by SEM images and the measurement of electrical conduction between indium electrodes. Indium electrodes are electron-beam deposited on ZnO nanorods array with 600 nm thick. Shape of anode is rectangular (4 mm x 4 mm) and that of cathode is triangular with 30 degree vertical angle and 3 mm base, and the separation between the side of anode rectangle and the vertex of cathode triangle is 1.5 mm.

DC voltage is applied between electrodes in vacuum. An electrical potential of the metal chamber is same as that of anode. It is gradually increased from 0 volt. When the applied voltage is low, electric current does not flow. When it reaches about 1500 V, however, the current of about 10<sup>-6</sup> [A] initiates abruptly to flow and bluish-white light emission is observed at many points along the cathode edge. These beams of light extend along lines with directions nearly vertical to cathode edge as if the anode electrode did not exist or the voltage was not applied on anode. The intensity of emitted light is very high. It is confirmed experimentally that electrons are field-emitted from ZnO nanorods being at the cathode edges and the light beams correspond to trajectories of the field-emitted electrons. We estimate that the light may be generated by collisions of these electrons with ZnO nanorods, and are studying on this mechanisms.

**NM-TuP7 Carbon Nanotube and Graphene Hybrid Thin Film for Transparent Electrodes and Field Effect Transistors, *Ki-Seok An, W. Song, S. Myung, J. Ihm,*** Korea Research Institute of Chemical Technology, Republic of Korea

Low-dimensional  $sp^2$  carbon materials including single-walled carbon nanotubes (swCNTs) and graphene have recently received a great deal of attention for potential uses in transparent and flexible nanoelectronics due to their remarkable mechanical, electrical, thermal, and optical properties. Especially, there are many interest in hybrid nanostructures including swCNTs and graphene. Here, we combined swCNTs and graphene hybrid films with complementary properties for use in high-performance transparent electrodes and field effect transistors (FETs). The hybrid films were synthesized by thermal chemical vapor deposition on Cu foil spin-coated with swCNTs. The density and alignment of swCNTs were simply controlled by adjusting the spin-coating speed or swCNT concentration. Evidence for the formation of the hybrid film was provided by the combined G- and 2D-bands intensity and lineshape Raman features of swCNTs and graphene. Based on the transfer characteristics for the hybrid film-based FETs, an improved  $I_{on}/I_{off}$  and on-state current are achieved compared with pristine graphene. Notably, the hybrid film had a sheet resistance of 300  $\Omega/sq$  with 96.4% transparency, which was comparable to that of hybrid materials in previous reports.

**NM-TuP9 Electrical Properties of Vertically Integrated Thin Film Transistors using Amorphous- $In_2Ga_2ZnO_7$  Channel Layer, *UnKi Kim, S.H. Rha, J.S. Kim, E.S. Hwang, S.J. Lee, Y. Jang, C.S. Hwang,*** Seoul National University, Republic of Korea

Recently, serially connected transistors with vertical configuration have received considerable attention in memory applications due to their potential to increase integration density to ultra-high values. In transistors with the vertically integrated configuration, the semiconductor channel material is usually composed of polycrystalline Si (poly-Si). Although the poly-Si channel has revealed feasible functionality as the semiconductor channel, degraded mobility, uniformity and reliability concerns related to the presence of grain-boundaries have not yet been completely resolved. In this regard, the amorphous nature and high carrier mobility of  $In_2Ga_2ZnO_7$  (a-IGZO) thin films attract a great deal of attention as the channel material for such applications.

In this study, two serially connected and vertically integrated a-IGZO thin film transistors (V-TFTs) were fabricated using a gate-first fabrication process. The V-TFTs were fabricated with a vertical channel length ( $L_g$ ) of  $\sim 500$  nm for the top TFT (t-TFT) and  $\sim 400$  nm for the bottom TFT (b-TFT). Heavily doped p-type silicon was used as the substrate and gate of b-TFT ( $G_b$ ). A 100-nm-thick  $SiO_2$  layer was thermally grown as the isolation layer between the t- and b-TFTs. 500-nm-thick poly-Si was deposited by low-pressure chemical vapor deposition to make the gate of the t-TFT ( $G_t$ ). Then, the poly-Si/ $SiO_2$ /Si structure was dry etched sequentially to form the gates. Then, a 100-nm-thick  $SiO_2$  layer was deposited by a PECVD as the gate dielectric layer, and an a-IGZO layer was sputter-deposited at room temperature on this structure with a target thickness of 100 nm on the top surface of the sample, which results in a channel thickness of  $\sim 40$  nm for the t-TFT, and  $\sim 50$  nm for the b-TFT on the side walls of the  $SiO_2$ . Finally, the Ti source and drain contacts were fabricated by a lift-off process, as the Ti contact with the a-IGZO is quasi-Ohmic.

The t- and b-TFTs show well-behaved transfer characteristics, with an  $I_{on}/I_{off}$  ratio ( $\sim 10^8$ ) and an SS value of 0.6 V/dec., which are much improved device parameters compared with the previously reported single-layer V-TFT, for which the gate-last fabrication process was adopted. This is due to the favorable distribution of the electric field by the  $V_d$  and  $V_g$  of the TFTs, where the influence of  $V_d$  on the channel can be minimized compared with that from  $V_g$ . While the two serially connected TFTs behave well and rather independently of each other, there were certain cross-influence between them. Details for such cross-talk will be discussed in the presentation. Further study results up to four layer V-TFT will also be presented.

**NM-TuP10 Synthesis and Application of Large-Area Transition Metal Dichalcogenides by Chemical Vapor Deposition, *Chong-Yun Park, Y.Kim, Kim, J.S.Kim, Kim, S.-H.Park, Park, Y.H.Ko, Ko,*** Sungkyunkwan University, Korea, Republic of Korea

Transition metal dichalcogenides ( $MoS_2$ ,  $WS_2$ ,  $WSe_2$ ,  $MoSe_2$ ,  $NbS_2$ ,  $NbSe_2$ , etc.) are layered materials that would exhibit semiconducting, metallic and even superconducting behavior. In the bulk, it is semiconducting and has an indirect band gap. Recently, these layered systems have attracted a great deal of attention mainly due to their complementary electronic properties when compared to other two-dimensional materials, such as graphene (a semimetal) and boron nitride (an insulator). However, these bulk properties could be significantly modified when the system becomes mono-layered; the indirect band gap becomes direct. Such changes in the band structure when reducing the thickness of a  $MoS_2$  and  $WS_2$  films has important

implications for the development of novel applications, such as valleytronics. In this work, we report for the controlled synthesis of large-area ( $\sim cm^2$ ) single-, bi-, and few-layer  $MoS_2$  and  $WS_2$  using a two-step process.  $MoO_x$  and  $WO_x$  thin films were deposited onto a Si/ $SiO_2$  substrate, and these films were then sulfurized under vacuum in a second step occurring at high temperatures (750  $^\circ C$ ). The synthesized  $MoS_2$  and  $WS_2$  atomic thin films were analyzed by optical microscopy, Raman spectroscopy and TEM, and their photoluminescence properties were evaluated.

**NM-TuP11 Bolometers of Aligned Carbon Nanotubes, *G. Garcia Valdivieso, Hugo R. Navarro Contreras, F.J. González,*** Coordinación para la Innovación y la Aplicación de la Ciencia y la Tecnología (CIACyT-UASLP), Mexico, *M. Quintana Ruiz,* Instituto de Física (IF-UASLP), Mexico, *G. Vera Reveles,* Coordinación para la Innovación y la Aplicación de la Ciencia y la Tecnología (CIACyT-UASLP)

The objective of this work is to report on a study on the preparation of bolometers and their characterization, based on parallel linear arrays of carbon nanotubes (CNTs).

The CNTs present good thermal and electrical properties. That is the reason why they may constitute competitive bolometric devices. A bolometer is a device that absorbs energy, in our case infrared radiation, thus varying its temperature (increasing) and electrical resistance (decreasing). The figure of merit of the bolometers is the temperature coefficient of resistance (TCR).

With the objective of obtaining aligned arrays of CNTs we made a solution in water with polymer (PVP), surfactant (SDBS) and CNTs. For a second group Functionalization was also performed with amino groups (Thymine) to induce better alignment, taking advantage of the hydrogen bonds that form between them.

For both sets of prepared CNT's copper was evaporated on them to have proper ohmic metal contacts to characterize the bolometers thus created.

The samples morphology and alignment were characterized by Scanning Electron Microscopy (SEM). Kaiser Test was performed to check on the degree of functionalization. The TCR of the constructed bolometers was electrothermally measured.

The results obtained with SEM were in some case alignments as long as 3 mm in length. The functionalization degree obtained was 1100  $\mu mol/g$ . We obtain values of TCR in the range of -1.7 to -3.0  $\% K^{-1}$  for non-functionalized CNTs and from -0.4 to -5.4%  $K^{-1}$  for functionalized CNT's. These last values are the largest reported for CNTs so far in the literature.

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**NM-TuP13 Mechanical Deformation in Si/ge Quantum Dots, *José Luis González Arango,*** Universidad de Pamplona, Colombia, *P. Freitas Gomes,* Universidade Federal de Goiás, Campus Jataí, Brazil

Mechanical deformation (strain) plays an important role in the electronic, optical and transport properties of semiconductor quantum dots (SQDs). Epitaxial SQDs have a spatial deformation profile caused by the mismatch of the lattice parameters of the materials involved. This deformation creates an elastic energy which is one determinant fact in the SQDs grown on Stranski-Kastranow mode. The deformation also changes the potential profiles experienced by the carriers (electron and hole), requiring consideration of them when one calculates the electronics eigenstates. This shows the importance of the deformation profile on the properties of the nanostructures for future applications in electronic and optical devices.

In this work we show one more tool for the calculation of mechanical deformation on Si/Ge semiconductor quantum dots. We used a numerical simulation package to solve the differential equations for the deformation, using Continuous Elasticity Theory. We studied two systems: capped and uncapped. The cap layer is the Si layer grown above the Ge QDs layer. On the capped system, we observed a larger biaxial deformation on the Ge layer plane, when compared with the uncapped system. We also observed the deformation on the Si layer underneath the Ge layer. Again, on the capped system this biaxial deformation was also larger. With these deformation profile, we can also calculate the stress tensor and the elastic energy profiles.

**NM-TuP14 Synthesis of Pt-based Bimetallic Nanoparticles using Pulsed Plasma Discharge in Water, SangYul Lee, Korea Aerospace University, Republic of Korea, S.M. Kim, Korea Aerospace University, Kora, J.-W. Kim, InCheon University, Korea**

The synthetic approach for electrocatalysts is one of the most important methods determining the electrocatalytic performance. In this work, we synthesized Pt and Pt-M (M=Cu, Ag, and Pd) bimetallic nanoparticles using a pulsed plasma discharge in water. A morphological investigation revealed that the as-synthesized Pt and Pt-M bimetallic nanoparticles constituted a nanochain network structure interconnected with primary nanoparticles, and the nanochains grew from the primary nanoparticles via the oriented attachment. The Z-contrast, EDX line scanning, and XRD analysis confirmed that the Pt was alloyed with M without elemental segregation or phase segregation. Furthermore, it was found that the composition difference was dependent on the electrode temperature determined by the power density and thermal parameters. The Pt-Pd bimetallic nanoparticles showed the largest electrochemical surface area due to a crystalline size of less than 5nm, whereas the Pt-Ag bimetallic nanoparticles showed superior electrocatalytic activity, stability, and durability with respect to the methanol oxidation reaction, which could be attributed to the downshift of the d-band center via electronic modification.

**NM-TuP15 Crystal Structure and Surface Orientation dependence of Hydrogen Adsorption on Iron Surfaces, Yuji Kunisada, Hokkaido University, Japan, N. Sakaguchi, Hokkaido University**

#### Introduction

In order to utilize hydrogen as new clean energy resources, we have to realize safe, efficient, and low cost hydrogen transportation and storage. One of the current transport methods is the one with high-pressure hydrogen tanks. However, hydrogen is one of the most important elements in the damage process of materials. Many recent studies have reported that hydrogen atoms absorbed in materials can stabilize vacancies[1], which cause reduction of their ductility. From this point, the atomic- and electronic-scale understanding of hydrogen embrittlement process is necessary to develop new long-life materials for hydrogen transportation and storage.

#### Calculation Methods

In this study, we investigated the adsorption properties of hydrogen isotopes on iron surfaces with the aid of first principles calculations based on spin-polarized density functional theory, in order to understand hydrogen behaviors in commonly-used iron-based materials, for instance, ferritic and austenitic stainless steels. We also adopted the quantum mechanics calculations of hydrogen nuclei, because the importance of delocalization and zero-point energy of hydrogen nuclei has been reported in various papers. [2, 3] Furthermore, we considered hydrogen(H), deuterium(D), tritium(T), and muonium( $\mu^+$ -e) as hydrogen isotopes.

#### Results and Discussion

At first, we investigated the potential energy surfaces of hydrogen on bcc-Fe(110) and fcc-Fe(111) surfaces. These surface orientations are the most stable ones for each crystal structure, respectively. Furthermore, in order to reveal the surface orientation dependence of hydrogen adsorption, we investigated the potential energy surfaces of hydrogen on fcc-Fe(100) surfaces. We revealed that the most stable adsorption sites on bcc-Fe(110), fcc-Fe(111), and fcc-Fe(100) surfaces are the long-bridge, fcc-hollow, and short-bridge site, respectively. The corresponding adsorption energies with these adsorption configurations are 2.99, 2.78, and 2.82 eV, respectively. Thus, we can point that the adsorption energies on bcc-Fe(110) and fcc-Fe(100) surfaces are slightly larger than the one on fcc-Fe(111) surfaces. We also investigated the hydrogen adsorption states on these surfaces by calculating schrödinger equation for hydrogen nuclei. We found the delocalization of H atoms in the ground state. In addition, we clarified the non-negligible isotope effects in delocalization and zero-point energy of hydrogen isotopes.

#### References

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**NM-TuP16 Synthesis and Evaluation of Nanocrystalline Diamond Powder Prepared by Coaxial Arc Plasma Gun, Hiroshi Naragino, A. Tominaga, Kyushu University, Japan, K. Sumitani, Kyushu Synchrotron Light Research Center, Japan, S. Hattori, Kyoto Prefectural Technology Center for Small and Medium Enterprises, Japan, T. Yoshitake, Kyushu University, Japan**

Diamond possesses several superior physical properties including high hardness, wide bandgap, and chemical inertness. Furthermore, it is possible

to impart functionalities by doping and surface modification. Nano-sized diamond powder shows different properties from bulk diamond. Nanodiamond has mainly been produced by detonation method so far. However, high-purity nanodiamond powder has been difficult to be fabricated by detonation. Moreover, the functionalization of nanodiamond is made after growth, because of *in-situ* doping being impossible. Our research group has proposed a new novel method that employs a coaxial arc plasma gun (CAPG), which enables us to fabricate nanodiamond crystallites. The specifics to this method are as follows: i) the growth is made using a simple apparatus equipped with a coaxial arc plasma gun, ii) high-purity nanodiamond can be fabricated in principle, iii) doping can be easily made by using doped targets, and iv) the grain size is expected to be changed by controlling the discharge condition of coaxial arc plasma gun. In this work, we experimentally proved the generation of nanodiamond by powder X-ray diffraction (XRD) and transmission electron microscope (TEM) and that the grain size is evidently enlarged with the electric power applied to an arc plasma gun. Moreover, the density of nanodiamond powder was measured using a sink-float method. Nanodiamond powder was fabricated using CAPG (ULVAC, APG-1000) equipped with a graphite target. The inside of the chamber fitted with CAPG was evacuated to  $< 10^{-6}$  Pa and hydrogen was introduced at 5 sccm. The head of the arc plasma gun was pointed at quartz plate heated at 550deg. C. The powder that quickly and automatically exfoliated from the quartz plate was gathered in the collection cell located under the quartz plate. In order to confirm the formation of diamond, the films were structurally investigated by TEM and powder XRD using synchrotron radiation at beamline 15 of the SAGA-LS. The films exhibited diamond-111 and -220 diffraction rings in the electron diffraction patterns and the existence of diamond grains was confirmed from the dark-field TEM images. The XRD patterns also exhibited diffraction peaks due to diamond. The grains size was increased from 2 to 80 nm with increasing electric power applied to an arc plasma gun. From the density measurement, the density of nanodiamond powder was estimated to be approximately 1.77 g/cm<sup>3</sup>. This value is smaller than that of diamond (3.5 g/cm<sup>3</sup>), and indicates that the nanodiamond contains the non-diamond phase such as an amorphous carbon. The details of preparation apparatus and preparation mechanism are explained in the conference.

**NM-TuP17 Surface Structure and Local Valence Electronic States of Si(110)-16x2 Surface after Exposure to Water: XPS and Auger-Photoelectron Coincidence Study, Takuhiro Kakiuchi, S. Nishiura, J. Kawamoto, Ehime University, Japan, S. Nagaoka, Ehime University, K. Mase, KEK, Japan**

Si(110)-16x2 is a favorable candidate for a next-generation semiconductor substrate because it takes a single domain (SD) structure with high hole-mobility, which is larger than that of the other Si crystal faces. Recently, Adatom-Buckling (AB) model has been proposed as the surface structure model for clean Si(110)-16x2 surface [1]. The AB model consists of five Si surface components of SC1: the buckled upper atoms, SC2: the unbuckled atoms and the second layer atoms with dangling bonds (DBs), SC3: the first layer and second layers atoms without DBs, SC4: the adatoms, and SC5: buckled lower atoms. In the AB model, the surface states  $S_1$ ,  $S_2$ ,  $S_3$ , and  $S_4$  with binding energies of 0.2 eV, 0.4 eV, 0.7 eV, and 1.0 eV are reported to be located at specific surface sites of SC4, SC1, SC5, and SC3, respectively [1]. However, the SD structure of Si(110)-16x2 disappears when it is exposed to atmospheric air. In this study, we investigated a water-terminated Si(110)-16x2 SD surface with XPS and Auger-photoelectron coincidence spectroscopy. Si-2p photoelectron spectra indicate that water is dissociatively adsorbed and forms Si-H and Si-OH components after exposure to water of 0.1 Langmuir (L). When Si(110)-16x2 surface is exposed to water from 1.0 L to 5.0 L, there is little change in these Si-2p intensity ratio. This result indicates that clean Si(110)-16x2 surface is saturated with water of less than 1.0 Langmuir (L). In addition, water is preferentially dissociative-adsorbed at surface components of the SC1, the SC2, and the SC3 on step edge of SD structure, but is hardly adsorbed at surface components of the SC4 and the SC5 on the terrace of the SD structure. The SD structure of Si(110)-16x2 surface after the exposure to water of 5.0 Langmuir is kept under ultra-high vacuums condition and atmosphere pressure of N<sub>2</sub> gas. This result indicates that Si(110)-16x2 SD surface is inactivated by water dissociative-adsorption. On the other hand, Si-L<sub>23</sub>VV-Si-2p coincidence spectra suggest that the surface states  $S_1$ ,  $S_2$ ,  $S_3$ , and  $S_4$  disappear after exposure to water. The valence band maximum energy of water adsorbed Si(110)-16x2 surface is shifted to deeper binding energy side in comparison with that of clean Si(110)-16x2 surface. The water adsorbed Si(110)-16x2 SD surface may be used as a unique semiconductor substrate.

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**NM-TuP19 Study on Tracking Resistance of Silicone Rubber Nanocomposite under DC Voltage.** *K.J. Lim, JungHun Kwon, J.S. Park,* Chungbuk National University Korea, Republic of Korea

One of the problems is tracking of outdoor polymeric silicone rubber (SIR) insulation used in HVDC or HVAC transmission lines. These problem are more serious with dc than with ac voltage, due to the electrostatic attraction of airborne contaminants to the insulator surface. In order to improve the tracking resistance of SIR, inclined plane (IP) tracking test similar to IEC 60587 was conducted under positive and negative dc voltages for SIR filled with micro sized silica and nano sized alumina trihydrate (ATH) fillers. The results show that tracking resistance of SIR nanocomposites were more increased than SIR unfilled micro or nano filler. It was also seen that the tracking resistance of SIR showed polarity effect under dc voltage.

**NM-TuP20 Decay Processes of Si 2s Core Holes in Si(111)-7×7 Revealed by Si Auger Electron Si 2s Photoelectron Coincidence Measurements,** *Kazuhiko Mase,* KEK, Japan, *K. Hiraga, S. Arai,* Yokohama National University, Japan, *R. Kanemura,* Yokohama National University, *Y. Takano, K. Yanase, Y. Ogashiwa,* Gunma University, *N. Shohata,* University of Tsukuba, *N. Kanayama,* Chiba University, *T. Kakiuchi,* Ehime University, Japan, *S. Ohno,* Yokohama National University, *D. Sekiba,* University of Tsukuba, *K. Okudaira,* Chiba University, *M. Okusawa,* Gunma University, *M. Tanaka,* Yokohama National University

The filling of an initial core hole by an electron from a higher subshell of the same shell is known as a Coster–Kronig transition, and Auger photoelectron coincidence spectroscopy (APECS), in which Auger electrons are measured in coincidence with photoelectrons with a fixed kinetic energy (KE), is an ideal tool for probing Coster–Kronig transitions because Auger electrons originating from a specific core ionization are detected.

However, studies of Coster–Kronig transitions have mainly been restricted to metal surfaces, even though Si surfaces are crucial for surface science applications and the semiconductor industry. Issues such as the assignments of the Si  $L_1VV$  Auger peaks, experimental determination of the branching ratio of the Si  $L_1L_{23}V$  and Si  $L_1VV$  Auger decays, and competition between the delocalization of the valence hole and the Si  $L_{23}V-VVV$  Auger decay are, to the best of our knowledge, largely unexplored. In this paper, we report on the decay processes of Si 2s core holes in a clean Si(111)-7×7 surface studied using coincidence measurements of the Si Auger electron and the Si 2s photoelectron.

We measured a coincidence spectrum measured by scanning the ASMA over a KE range of 20–150 eV, with the DP-CMA fixed at a KE of 76.5 eV (Si- $L_{23}VV$ -Si-2p APECS spectrum). Distinct Auger peaks are observed in a KE region of 50–92 eV with the maximum peak located at KE = 88 eV. We assigned these peaks to Si  $L_{23}VV$  Auger electrons emitted in the decay processes of Si 2p holes. Another coincidence spectrum was measured by scanning the ASMA over a KE range of 20–150 eV with the DP-CMA fixed at KE = 26.3 eV, which corresponds to Si 2s photoelectrons (Si-Auger-Si-2s APECS spectrum). The maximum peak position and shape of the Si-Auger-Si-2s APECS spectrum in the AeKE = 50–92 eV region are almost identical to those of the Si- $L_{23}VV$ -Si-2p APECS. Therefore, we assigned these Auger peaks to Si  $L_{23}VV$  Auger processes. This is direct evidence of Si  $L_{23}VV$  Auger processes being induced by Si 2s ionization.

The peaks of Si-Auger-Si-2s APECS in the AeKE = 20–50 regions were assigned to Si  $L_1L_{23}V$  Auger decays, while the peaks of Si-Auger-Si-2s APECS in the AeKE = 100–150 eV regions were assigned to Si  $L_1VV$  Auger decays. These results indicate that there are two nonradiative decay processes of the Si 2s core hole. The first is the Si  $L_1L_{23}V$  Coster–Kronig transition followed by delocalization of the valence hole and Si  $L_{23}VV$  Auger decay, while the second is Si  $L_1VV$  Auger decay. From the integrated intensity of the normalized Si  $L_{23}VV$  and Si  $L_1VV$  Auger peaks, we estimated the branching ratio of Si  $L_1L_{23}VV$  to Si  $L_1VV$  Auger processes to be  $(96.8 \pm 0.4):(3.2 \pm 0.4)$ .

**NM-TuP21 Pulsed Laser Assisted Synthesis of NaLa(MoO<sub>4</sub>)<sub>2</sub>:Ho<sup>3+</sup>/Tm<sup>3+</sup>/Yb<sup>3+</sup> Nanocrystals and their White Upconversion Luminescence,** *Jeong Ho Ryu, J.-I. Lee,* Korea National University of Transportation, Korea

In recent years, lanthanide ion doped upconversion (UC) luminescence from near infra-red radiation to visible or UV light has received many attention for their various applications in phosphors, solar cell, flat-panel displays, scintillators, solid state lasers and fluorescent bio-medicals. In the fields of industries, it is required that UC luminescent materials should be engineered to emit wide ranges of white colors. Also, high chemical, physical and mechanical stabilities should be achieved through engineering UC materials. Although multi-color UC luminescence with high efficiency was reported using lanthanide doped fluorides emitting bright blue emission of Tm<sup>3+</sup> and green or red of Er<sup>3+</sup> under laser excitation (980 nm), fluorides

can decompose easily with moisture in air which makes the application difficult in the fields of industries. Conventionally, solid state reaction, precipitation, hydrothermal and sol-gel methods were used for synthesis of nanocrystalline NaLa(MoO<sub>4</sub>)<sub>2</sub> particles. However, those methods need long processing time and steps for fabrication. Also, chemical additives in procedure may be incorporated to NaLa(MoO<sub>4</sub>)<sub>2</sub> particles as impurities, which results in bad influence to human body clinically. One novel technique for fabrication of NaLa(MoO<sub>4</sub>)<sub>2</sub> nanocrystals is pulsed laser ablation (PLA) in liquid medium. PLA of solid target in liquid has been a promising technique for producing nanocrystals for analytical and bioanalytical applications as well as the rapid synthesis of complex materials because the experimental procedure is simple and above all, chemical additive is unnecessary. However, to date, there is little report on the preparation of upconverting NaLa(MoO<sub>4</sub>)<sub>2</sub> nanocrystals by laser ablation in liquid medium. In this study, we report a novel synthetic approach to produce Ho<sup>3+</sup>, Tm<sup>3+</sup>, Yb<sup>3+</sup> tri-doped NaLa(MoO<sub>4</sub>)<sub>2</sub> nanocrystals using PLA in liquid medium without any surfactant. The fabricated NaLa(MoO<sub>4</sub>)<sub>2</sub>:Ho<sup>3+</sup>/Tm<sup>3+</sup>/Yb<sup>3+</sup> nanocrystals were characterized in terms of their crystallinity, microstructure and white upconverting property. Moreover, the laser ablation process was discussed by a thermally induced explosive ejection mechanism.

**NM-TuP22 DFT Study of Surface Passivation of Silicon Carbide Nanowires by Halogens,** *Miranda,* Universidad Nacional Autónoma de México, *Trejo,* Instituto Politécnico Nacional, México, *Cruz-Irisson, Luis A. Pérez,* Universidad Nacional Autónoma de México

The use of silicon carbide nanowires (SiCNWs) as chemical sensors stands out among their many possible applications. At present, SiCNWs are usually coated with SiO<sub>2</sub>. To further extend and customize their applications, surface modification of nanowires (NWs) by different chemical species is one of the feasible ways to achieve it. An insightful understanding of the effects of such passivating functional groups is thus important to understand the electronic properties of surface modified NWs. In this work, by using density-functional calculations, we study the stability and the electronic structure of SiCNWs passivated with halogen atoms such as F, Cl, Br or I, considering different surface covering schemes. We show that the stability of SiCNWs strongly depends on both the passivating element and the percentage of surface covering, in an otherwise fully hydrogen passivated NW. Moreover, when going from the most stable system to the less stable one, the following stability trend is obtained: F-SiCNW > Cl-SiCNW > Br-SiCNW > I-SiCNW > H-SiCNW, which can be attributed to the different electronegativities of the passivating elements considered. Finally, the effects of chemical decoration on the size and nature of the NW band gaps are discussed.

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