Nano and 2D Materials
Room Naupaka Salon 1-3 - Session NM-WeP
Nano and 2D Materials Poster Session

NM-WeP-1 Introduction to Measurement Uncertainty Evaluation Method and Results of Silicon Nitride Thin Film Layer Thickness and Complex Dielectric Constant, ***Yong Jai Cho***, *W. Chegal,* Korea Research Institute of Standards and Science, Republic of Korea

SE (Spectroscopic Ellipsometer) has excellent measurement resolution, but measurement quality control of SE requires careful attention because measurement uncertainty can be easily affected by small changes in the device. For SE measurement quality control, thin film layer thickness certified reference materials are mainly used. SE has the advantages of being non-destructive, ultra-fast, and non-contact, but also has excellent high-precision characteristics that can detect a single atomic layer even before it is completely grown, so demand is increasing as a core measurement equipment for the semiconductor device manufacturing process. As semiconductor device manufacturing technology has recently developed due to the complexity of semiconductor device structures, the introduction of atomic layer-level processes, and the introduction of new materials, there is a need to improve quality control of TTTM (Tool-To-Tool Matching) related to measurement uncertainty. Therefore, in order to improve the measurement quality control level of SE equipment for semiconductor processing, it is necessary to develop higher quality thin film layer thickness certified reference materials. As a first research step, our research team developed a unified uncertainty evaluation method for the measurands of various types of rotating-element spectroscopic ellipsometers with excellent real-time measurement performance[1]. This method allows the measurement uncertainty of ellipsometric transfer quantities (e.g. Psi and Delta) to be calculated directly from observed ellipsometric transfer quantities, so there is no need for the analysis results of unknown optical properties of the sample required to calculate the measurement uncertainty. As a second research step, we developed a method for assessing uncertainty in the values of unknown optical properties of the sample, obtained using a nonlinear least-squares fit from the spectra of the observed ellipsometric transfer quantities[2]. The implicit function theorem was adopted to describe the propagation of uncertainty for nonlinear least-squares calculations[3]. We would like to introduce the method and results of applying the developed uncertainty evaluation method to the uncertainty evaluation of the thin film layer thickness and complex dielectric constant of silicon nitride thin film sample obtained through SE.

References

[1] Y. J. Cho, W. Chegal, J. P. Lee, and H. M. Cho, Opt. Express **24** 26215 (2016).

[2] Y. J. Cho and W Chegal, Opt. Express **29** 394428 (2021).

[3] J. A. Fessler, IEEE Trans. Image Processing **5**, 493 (1996).

NM-WeP-2 A New Tool for Single Ion Implantation and Nanoscale Materials Engineering: System Design and Source Development, ***Paul Blenkinsopp***, Ionoptika Ltd., UK*; K. McHardy,* Ionoptika, Ltd., UK*; G. Aresta,* Ionoptika Ltd., UK

Quantum computing is the next great frontier of science. It has the potential to revolutionize many aspects of modern technology, including digital communications, “quantum-safe” cryptography, and incredibly accurate time measurements.

Single impurity atoms in semiconductors are receiving attention as potential quantum technologies, and proof-of-concept devices have shown promise. However, such devices are incredibly challenging to manufacture, as single atoms must be placed within ~ 20 nm of each other within a pure ^{28}Si matrix.

All working devices thus far have been fabricated using hydrogen lithography with an STM followed by atomic layer deposition. This is labour-intensive and requires several days of meticulous preparation to create just a single quantum bit (qubit). Real-world devices will require arrays of hundreds or thousands of impurity atoms, highlighting the requirement for a scalable method of positioning single atoms with nanometer precision.

We report on a new commercial instrument for the fabrication of quantum materials and devices via single ion implantation.

The instrument features a high-resolution mass-filtered focused ion beam (FIB), a high-sensitivity deterministic implantation system, 6-inch wafer handling, and a high-precision stage. The deterministic implantation system allows single ion implantation with confidence levels as high as 98%.

The ion dose delivered to the sample can be adjusted across a wide range, providing many nanoscale materials engineering capabilities in a single tool, from single ion implantation to direct-write capabilities such as isotopic enrichment and targeted ion-implantation of nanomaterials.

The liquid metal alloy ion sources, coupled with and mass filtered column will enable for the implantation of many different elements with isotopic resolution. Available sources include silicon, erbium, gold, and bismuth, while many others of technological interest are in development. We will report on the LMIG source development carried out at Ionoptika in collaboration with our partners.

NM-WeP-3 Graphene-Incorporated Dielectric Composites by Varying the Mixing Method and Degree of Oxidation of Graphene, *S. Jun,* ***Kwangsin John Ahn***, *S. Yu,* Hankuk University of Foreign Studies, Republic of Korea

Graphene-incorporated dielectric composites by varying the mixing method and degree of oxidation of graphene

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To obtain high-performance dielectric properties of dielectric composites, graphene and barium titanate ($BaTiO_3$, BTO) fillers were mixed in the polymer matrix, by varying the degree of reduction of graphene and the mixing method. Two kinds of graphene materials, i.e., graphene oxide (GO) and reduced graphene oxide (rGO); and two kinds of mixing methods for graphene and BTO, i.e., encapsulation of BTO in graphene and subsequent mixing, and simple mixing of BTO and graphene in the polymer matrix. This yielded to four kinds of graphene-incorporated samples, which was compared with the reference sample, i.e., a sample with only BTO fillers in the polymer matrix without graphene. Encapsulation process was performed by the self-assembly of positively functionalized BTO and negatively functionalized GO. After the encapsulation, GO-encapsulated BTO fillers were chemically reduced to become rGO-encapsulated BTO fillers [1,2]. All the four graphene-incorporated samples exhibited better dielectric constant values, i.e., 1.5 to 2.2 times higher than the reference sample. It was thoughted to be caused by the presence of graphene via the interfacial polarization or micro-capacitor effects [1]. However, the increase in dielectric loss, which had frequently occurred for the simple mixing cases of conducting nano-fillers, was successfully suppressed for the encapsulated samples. Here, the dielectric loss was controlled under lower 20%, which was caused by removal of free graphene platelets during the chemical process of the encapsulation [2]. The best performance one is the encapsulation method for rGO material. The next one is GO encapsulation case. The highest enhancement of 120% in the dielectric constant and moderate dielectric loss was obtained for rGO-encapsulation case. Therefore, we can say that encapsulation of BTO in graphene is very promising mixing method for high-performance polymer-based dielectric composite materials.

References:

[1]S.-Y. Jun et al., Carbon **199**, 23 (2022).

[2]S.-Y. Jun et al., Mater. Chem. Phys. **255**, 123533 (2020).

NM-WeP-4 Deep Learning-Based Prediction of Adsorption Energies for MoO_2Cl_2 Precursor on SiO_2 Surface Using Density Functional Theory, ***Do-Hyun Kwon***, *J. Lee,* Korea University of Technology and Education, Republic of Korea*; J. Kim,* Pohang University of Science and Technology (POSTECH), Republic of Korea*; Y. Kim,* Korea University of Technology and Education, Republic of Korea

A search for appropriate adsorption geometries of a MoO_2Cl_2 precursor on an -OH terminated β-SiO_2 surface was conducted using a deep-learning approach. The adsorption geometries were configured by translating and rotating the precursor located near the surface. A deep-learning model was developed to learn important properties of the adsorption geometries; the model consists of three main units to learn positional features of the precursor atoms, to learn distance features among the precursor and surface atoms, and to predict the corresponding adsorption energy. A dataset of adsorption geometry and the adsorption energy pairs was collected by grid search. Using this dataset, the model was trained to predict the adsorption energies with minimal error and optimized to achieve a root mean square error (RMSE) of less than 0.011%. Energetically more favorable adsorption geometries were found using the trained model. By inputting arbitrary adsorption structures into the trained model and

obtaining the predicted adsorption energies, recommendations for energetically stable adsorption structures were received. Through actual calculations, it was confirmed that the model could identify energetically stable adsorption structures that were not included in the dataset. The proposed method is applicable to finding appropriate adsorption geometries of other types of precursors and surfaces.

NM-WeP-5 Induced Self-Assembly of Small (3 - 5 nm) Nanoparticles Into Flexible Nanofilms at Air- and Oil-Water Interfaces, *H. Cameron, Y. Zhang, K. Leslie, B. Scott, I. Curtis, L. Gamble,* ***M.-Vicki Meli,*** Mount Allison University, Canada

Thin-film assemblies of gold nanoparticles (AuNPs) at the liquid interfaces have been an exciting research area over the past decade due to their promising applications in optics, sensors, shape-shifting and meta-materials, and catalysis. Autonomous self-assembly at such interfaces is an attractive method of synthesizing these superstructures, however this is a complex process that has proven to be difficult to control. Small AuNPs with core sizes <10 nm pose greater difficulties than larger AuNPs because they have a small free energy of adsorption that is comparable to their thermal energy. Therefore, there are few published examples of the self-assembly of such AuNPs at the liquid-liquid interface. The present research analyzes the effects of various experimental parameters on the adsorption of ~3 nm AuNPs to the oil–water interface, including ligand shell composition, alcohol additive structure and amount, oil phase composition and the phase of NP introduction. Film quality is qualitatively assessed and compared with a recent thermodynamic model to elucidate the primary driving forces of adsorption. Films with tunable optical density ranging from lightly coloured to gold and lustrous, are obtained with variation over a single parameter. Determining approaches that promote the adsorption of 3 nm AuNPs to an aqueous interface and furthering the understanding of its thermodynamic mechanism is necessary to gain precise control and to work towards the industrial use of such thin films.

NM-WeP-6 Molecular Structure and Vapor Pressure of Molybdenum Pentachloride Using Ab-Initio Thermodynamics, *N. Lee,* Korea University of Technology and Educaiton, Republic of Korea*; S. Kim, J. Kim,* ***Yeong-Cheol Kim,*** Korea University of Technology and Education, Republic of Korea

This study aims to elucidate the molecular structure and vapor pressure of molybdenum pentachloride in the gas phase using ab-initio thermodynamics. Molybdenum pentachloride can exist as $MoCl_5$ (monomer) and/or Mo_2Cl_{10} (dimer). The monomer is thermodynamically favored above 215 K, but Cl-Cl bond breakage is required to dissociate a dimer into two monomers. This suggests that the dimer is kinetically favorable even above 215 K, and the calculated dimer vapor pressure agrees well with the experimental data.

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