MM 63: Nanomaterials II

Time: Thursday 12:00–13:30 Location: IFW D

MM 63.1 Thu 12:00 IFW D

Nanoplasmonics from large-scale ab initio calculations: opposite trends in Ag and Na clusters — •Marc Barbry[1], Peter Koval[2], Natalia E. Koval[1], Javier Aizpurua[1], and Daniel Sánchez[1,2] — [1]Material Physics Center, San Sebastián, Spain — [2]Donostia International Physics Center, San Sebastián, Spain

An accurate description of electronic excitations is indispensable for understanding material properties and designing nanoscale devices. For instance, using large-scale TDDFT calculations, we have recently demonstrated the importance of taking into account the details of the atomic-scale structure [1] and the quantization of electron transport [2] in metal nanostructures in order to accurately describe their plasmonic properties. In this contribution we will compare the surface plasmon resonance of sodium and silver clusters within the same framework of *iterative* TDDFT [3]. Recent progress in our implementation made it possible to perform calculations of large clusters of diameters ranging from a few Å to 4–5 nm, counting up to 5000 silver atoms and using only modest computational resources (a 32-core node with 500GB RAM). With these new capabilities, we have characterized the size-scaling of the SPR frequency for both sodium and silver clusters. As expected these two materials show opposite behaviours that can be related to the different spill out of charge at the surface and to the additional screening created by the 4*d* electrons in silver.

[1] M. Barbry *et al. Nano Letters*, **15** (2015) 3410. [2] F. Marchesin *et al. ACS Photonics*, **3** (2016) 269. [3] P. Koval *et al. J. Phys.: Condens. Matter*, **28** (2016) 214001.

MM 63.2 Thu 12:15 IFW D

Ein-Photon-Ein-Elektron-Resonanz zur Interpretation der Spektren formanisotroper Nanopartikel aus mikrofluidischer Synthese — •Michael Köhler, Danja Kuhfuss und Andrea Knauer — TU Ilmenau, Inst. für Mikro- und Nanotechnologien

Die kontinuierliche tropfenbasierte mikrofluidische Synthese liefert Gold- und Silbernanopartikeln in verschiedenen Formen in sehr hoher Ausbeute und enger Größenverteilung. Durch Wahl der Konzentrationsverhältnisse der Reaktanden lassen sich Formen und Größen der Partikel und damit die optischen Resonanzen reproduzierbar einstellen. Untersuchungen an homogenen kolloidalen Lösungen von flachen Silberdreiecksprismen und Goldnanostäbchen zeigen, dass Größen- und Formeffekte auf die langwellige Absorptionsbande gut mit einer einfachen Beschreibung als 1-Photon-1-Elektron-Resonanz interpretiert werden können, was in Analogie zu molekularen Anregungsprozessen gesehen wird. Die langwelligen Absorptionsbanden der dimensionsreduzierten Partikel weisen auf Resonanzeigenschaften hin, die materialunabhängig sind und nur von der Partikelgeometrie bestimmt werden.

MM 63.3 Thu 12:30 IFW D

Single target sputter deposition of alloy nanoparticles with adjustable composition via gas aggregation cluster source — •Alexander Vahl[1], Julian Strobel[2], Wiebke Reichstein[1], Oleksandr Polonskyi[1], Thomas Strunskus[1], Lorenz Kienle[2], and Franz Faupel[1] — [1]Christian-Albrechts University at Kiel, Institute for Materials Science, Chair for Multicomponent Materials, Kaiserstr. 2, 24143, Kiel, Germany — [2]Christian-Albrechts University at Kiel, Institute for Materials Science, Chair for Synthesis and Real Structure, Kaiserstr. 2, 24143, Kiel, Germany

Over the past decades, noble metal nanoparticles were well studied regarding their catalytic and optical properties. Recently, alloy (noble) metal nanoparticles gained increased interest for their additional degree of freedom to tailor properties like particle plasmon polaritons. In this work we present a simple approach to prepare noble metal alloy nanoparticles with good control over size and size distribution as well as composition. Employing a Haberland type single DC magnetron gas aggregation cluster source with a multicomponent target, AgAu alloy nanoparticles with tunable composition were embedded into a SiO2 matrix (pulsed reactive DC sputtering). Nanocomposite analysis (TEM, UV-vis, XPS) revealed the possibility of concentration variation of about 15% and a corresponding shift of the plasmonic absorption band by about 20nm.

MM 63.4 Thu 12:45 IFW D

Towards Graphene synthesis: a comparative study of Nickel/SiO2/Si annealing in vacuum and hydrogen — •Fatima Akhtar[1], Grzegorz Lupina[1], Peter Zaumseil[1], Sebastian Schulze[1], Andre Wolff[1], Thomas Schroeder[1,2], and Mindaugas Lukosius[1] — [1]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]BTU Cottbus-Senftenberg, Konrad-Zuse Straße 1, 03046 Cottbus, Germany

In microelectronics, large area growth of high quality graphene is of highest importance. Metallic catalysts like Nickel (Ni) favors the synthesis of graphene by Chemical Vapor deposition (CVD). In the present study, we show the optimization of 200 nm Ni/SiO2/Si substrates for the growth of graphene. A series of annealing was performed in the temperature range (925-1050 *C) in either vacuum or hydrogen ambient. If Ni was annealed in vacuum conditions, it was thermally stable up to 1050 *C and smoother (rms = 10.3 nm) as compared to the rms value (48.5 nm) of the samples, annealed in hydrogen atmosphere. X-ray diffraction (XRD) spectra revealed the poly-crystalline structure of Ni, where mainly Ni (111) and Ni (200) reflections have been observed. The poly-crystallinity of Ni with the main Ni (111) orientation was also confirmed by the electron back scattering diffraction (EBSD) technique. In the final step, graphene was then deposited on the annealed Ni samples, using ethylene (C2H4) as a precursor gas (deposition time: 5 min at 1x10-2 mbar pressure and deposition temperature of 925 *C). Typical G and 2D peaks were identified in the Raman spectra, indicating good quality of graphene and large grains.

MM 63.5 Thu 13:00 IFW D

Thermal and Photothermal Reshaping of Gold Nanorods — •Phillip Witthöft[1], Christian Strelow[1], Tobias Kipp[1], Gerhard Grübel[2], and Alf Mews[1] — [1]Universität Hamburg, Institut für Physikalische Chemie, Hamburg, Deutschland — [2]Deutsches Elektronen-Synchroton, Hamburg, Deutschland

Gold nanorods are cylindrical structures of colloidal gold with very interesting optical properties because of their shape dependent plasmonic resonances. The location of these plasmonic resonances in their extinction spectrum hardly depend on the aspect ratio of the nanorods. Consequently, structural changes such as melting or surface rearrangement can be observed on the nanoscale following the location of the surface plasmon resonance. Here, we present different techniques to use thermal and photothermal energy to induce shape changes in gold nanorods even below the melting point. We use optical spectroscopy to track structural changes via the plasmonic resonances and compare them with transmission electron microscope images of the generated nanostructures. Based on our observation we discuss the possibilities of thermal reshaping on the nanoscale.

MM 63.6 Thu 13:15 IFW D

three dimensional image reconstruction from two dimensional image of TiO2 nanodevices — •Jesus Alan Calderon Chavarri[1], Min Zhou[2], and Yong Lei[3] — [1]TU Ilmenau, Ilmenau, Germany — [2]TU Ilmenau, Ilmenau, Germany — [3]TU Ilmenau, Ilmenau, Germany

This work describes a mathematical analysis to rebuild three dimensional (3D) image from two dimensional (2D) images of TiO2 nanodevices based on Anodic Alumina Oxide (AAO) templates, this yields to have an idea concerning part of nanodevices which can not be possible to see by figures captured by Scanning Electron Microscope SEM. For a further understanding of the mathematical analysis made in this work, it is designed simulation algorithms by MATLAB, also experiments in order to test simulation results.