DS 24: Layer Properties II: Optical Properties

Time: Wednesday 11:00–12:15 Location: CHE 91

DS 24.1 Wed 11:00 CHE 91

Theoretical description of optical properties in thin film materials — •Christine Giorgetti[1,2] and Valérie Véniard[1,2] — [1]Laboratoire des Solides Irradiés, CNRS, EcolePolytechnique, CEA/DRF/IRAMIS, Institut Polytechnique de Paris, F-91128 Palaiseau — [2]European Theoretical Spectroscopy Facility

In the framework of periodic boundary codes, the standard way to describe surfaces, or more generally isolated objects, is to build a supercell with vacuum, to separate the artificial replicas. We have shown that this procedure gives an absorption spectrum which depends on the vacuum introduced in the supercell.

We have proposed a new method called Selected-G to solve this vacuum problem. In TDDFT, it consists to solve the Dyson equation on a reduced set of reciprocal lattice vectors defined according to the thickness of the matter. During this derivation, we have evidenced a non-diagonal expression for the Fourier transform of the Coulomb potential, called slab potential. In the limit of an infinite thickness of matter, we recover the standard 3D expression of the Coulomb potential, and it has been successfully applied to describe optical properties for silicon surfaces.

In the case of electron energy loss (EEL), the vacuum problem also affects the in-plane components and the full expression of the slab potential in the Selected-G formalism is crucial to describe slabs of finite thickness, as it will be illustrated for few layers graphene slabs. These results open the question of the relationship between EEL and absorption spectra for thin slabs of matter.

DS 24.2 Wed 11:15 CHE 91

Highly reflective, stable mirror coatings for NIR and MIR spectral range by Atomic Layer Deposition — •Paul Schenk[1,2] and Adriana Szeghalmi[1,2] — [1]Fraunhofer-Institute for Applied Optics and Precision Engineering IOF, Center of Excellence in Photonics, Albert-Einstein-Str. 7, D-07745 Jena, Germany — [2]Friedrich-Schiller-University Jena, Institute of Applied Physics, Albert-Einstein-Str. 15, D-07745 Jena, Germany

Thin and smooth mirror coatings are essential for numerous optical systems in spectroscopy, astronomy, sensing, and lightning. Metallic reflectors cover from the ultraviolet to infrared a very broad spectral range. Well-established materials for highly reflective mirrors in the near (NIR) and mid (MIR) infrared spectral range are aluminum, silver, and gold. However, these materials degrade due to mechanical stress on the surface or thermal exposure, which leads to a decrease in reflectivity.

Iridium is a noble metal that has a reflectivity in the NIR and MIR spectral range similar to the established materials. It is very hard, extremely dense, chemically very stable and can be deposited as a smooth metal thin film by atomic layer deposition (ALD). It is scratch-resistant, abrasion-stable and thermally stable. Due to its enormously high melting point of over 2400 °C, it can even resist the highest temperatures. In the presented work, we studied the mechanical and thermal stability of iridium mirrors with regard to their reflectivity in the NIR and MIR spectral range.

DS 24.3 Wed 11:30 CHE 91

High resistive NbO_2 thin-films for phase-change switching applications — •Julian Stoever, Jos E. Boschker, Nazir Jaber, Saud Bin Anooz, Martin Schmidbauer, Jutta Schwarzkopf, Martin Albrecht, and Klaus Irmscher — Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany

Niobium dioxide has recently gained increased interest as it exhibits a semiconductor-metal transition together with a structural phase transition similar to that of vanadium dioxide. (VO_2). In contrast to VO_2, NbO_2 has phase transition temperature of 1080 K, which is well above room temperature and makes the material very interesting for resistive switching devices. We demonstrate the growth of single-crystalline $NbO_2(001)$ by pulsed laser deposition on $MgF_2(001)$ substrates. A subsequently performed annealing step results in a significantly sharper symmetric $NbO_2(004)$ x-ray diffraction peak and in a change of surface morphology. Ellipsometry, absorption spectroscopy and temperature-dependent resistivity measurements (TDR) were performed on the epitaxial layers. A single-crystalline NbO_2 bandgap energy of 0.89 ± 0.03 eV was consistently measured. This is in good agreement with density functional theory calculations by O'Hara et al. [J. Appl. Phys. 116, 213705 (2014)]. Furthermore, TDR were performed to determine deep level defects in the material. Finally, we will demonstrate first NbO_2 epitaxial layers on sapphire (Al_2O_3) substrates. Sapphire appeared to be more stable during the annealing, resulting in promising NbO_2 epitaxial layers.

DS 24.4 Wed 11:45 CHE 91

Metastability in Kesterite solar cells and dominant recombination process at open circuit voltage. — •Mbafan Samantha Lyam — Photovoltaics group, Martin Luther University, Halle-Wittenberg, 06120 Halle (Saale), Germany. — Department of Physics, Benue state University, Makurdi, PMB 102119, Nigeria.

kesterite solar cells (Cu2ZnSn(S,Se)4) have been investigated with the aim of determining meta-stability response and the dominant recombination path of the cells via open circuit voltage transients, admittance spectroscopy, capacitance voltage profiling techniques and current-voltage analysis. Exposure to red light was used to induce meta-stability and thereafter, the resulting slopes of the open circuit voltage transients, in combination with the diode quality factor and activation energy of the saturation current density obtained from fits of measured current-voltage curves, give insight into which region of recombination limits the cells at open circuit voltage.

DS 24.5 Wed 12:00 CHE 91

Tuning of Optical Properties in Highly Conducting Perovskites — •Mahdad Mohammadi, Aldin Radetinac, Thorsten Schneider, Alexey Arzumanov, Philipp Komissinskiy, and Lambert Alff — Institute of Materials Science, Advanced Thin Film Technology, Technische Universität Darmstadt, Darmstadt

The demand for transparent, conducting materials (TCMs) has skyrocketed in the past decades and will further increase due to the development and commercial success of devices like LCDs, capacitive touchscreens and OLEDs. For most TCM applications, doped wide-bandgap semiconductors like ITO (In_2O_3:Sn) are used due to the very good transparency in the visible. However, the conductivity in doped semiconductors is limited by the solubility of dopant elements. Recently, a new type of material has gained attention for application as TCM. The perosvkites SrMO3 (M = V, Mo, Nb) are all highly conducting, with $SrMoO_3$ ($\rho = 5.1\ \mu\Omega$cm) even surpassing the electrode material platinum. In addition, a moderately enhanced electron correlation reduces the plasma frequency ω_p and therefore induces transparency in large parts of the visible spectrum[1]. The scope of this work is to investigate the materials $SrVO_3$, $SrMoO_3$ and $SrNbO_3$ and related compounds to evaluate how and to what extend the properties can be manipulated towards desired characteristics. For this purpose, epitaxial thin films were deposited via pulsed laser deposition and characterized regarding structural, chemical, optical and electrical properties.

[1]A. Radetinac *et al.*, J. Appl. Phys., 119, 055302 (2016)