MM 16: Interfaces II

Time: Monday 16:15–17:00 Location: H5

MM 16.1 Mon 16:15 H5

Novel molecular dynamics potential for hybride metal-carbon systems — •Leonhard Mayrhofer and Michael Moseler — Fraunhofer IWM, Wöhlerstrasse 11, 79108 Freiburg

Nanomaterials based on sp^2-hybridized carbon like graphene and carbon nanotubes are objects of intense study due to their high potential for applications and their unique physical properties. But in most cases not pure all-carbon systems are of interest. E.g. for electronic or catalytic applications the carbon systems will generally be combined with metals. Therefore the aim of our work is an improved atomistic modelling of the interfaces in hybride carbon-metal-systems.

So far pair potentials are frequently used to model the interaction between carbon and metal atoms in molecular dynamics (MD) simulations [1-3]. However, this approach cannot be conciled with ab-initio calculations of various metal clusters (e.g. Al,Pd) on graphene showing a significant dependence of the metal-carbon bonding strength on the metal coordination.

We present a MD-potential in the spirit of the embedded atom method [4] giving a unified description of metal-carbon and metal-metal interactions capable of treating different metal coordinations at the same time. We apply this potential to determine realistic structures of contacts between metals and carbon nanosystems.

[1] S.Duffe et al., Euro. Phys. J. D **45**, 401 (2007)
[2] W.Y. Choi et al., Phys. Rev. B **68**, 193405 (2003).
[3] S.K.R.S. Sankaranarayanan et al., Phys. Rev. B **72**, 195405 (2005).

MM 16.2 Mon 16:30 H5

Finite element calculations of surface enhancement in attenuated total reflection infrared spectroscopy — •Ganesh Vasan and Andreas Erbe — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Surface Enhanced Infrared Absorption Spectroscopy (SEIRAS) is an effective tool at studying organic molecules in contact with metal nanostructures. Roughness or tailored structures on metal surfaces give rise to surface enhancements in the absorption spectra. A finite-element based solver of the Maxwell equations was used to simulate full spectra of organic molecules in contact with spherical and cylindrical nanostructures in the Attenuated Total Reflection (ATR) geometry on silicon internal reflection elements. Surface enhancement factors are defined, as obtained through reference runs.

The simulated field images and the absorption spectra show enhancements in both isolated and periodic cases with the absorbance increasing with decreasing inter-particle spacing. The computations confirm the experimental evidence that closer particles yield larger enhancements. Effects due to particle size have also been analysed, where larger particles show larger enhancements. The field images suggest the enhancement is because the particles act as local cavities.

MM 16.3 Mon 16:45 H5

Dielectric anti-reflective coatings for attenuated total reflection spectroscopy through metal films — •Martina Reithmeier and Andreas Erbe — MPI für Eisenforschung, Düsseldorf, Deutschland

In order to obtain insight into structural transformation during an electrochemical reaction, attenuated total reflection (ATR) infrared spectroscopy has proven to be a useful tool. The applicability is, however, limited when applied on continuous metal films, because of the metal's high reflectivity. In order to overcome this limitation, we introduce a novel system of stratifications. On the incidence media (silicon, calcium fluoride or zinc selenide), a thin layer of germanium with a thickness $\sim$1 μm is evaporated, followed by a 20 nm gold layer.
For certain wave numbers the reflectivity of the system is significantly lowered compared to a reference system. Calculations show that a higher absorption of the investigated material is expected at these wavenumbers. Experiments based on calculations were performed on Si-Ge-Au-H_2O, CaF_2-Ge-Au-acetonitrile and ZnSe-Ge-Au-acetonitrile and -acetone systems. In acetonitrile, a splitting of most vibrational absorptions is observed in contact with gold, which could originate from the strong interaction with gold.
The experiments so far show qualitative agreement with the computations. The regions with lower reflectivity are found and can be modelled. They show a strong sensitivity towards the presence of material close to the interface. Current problems are holes in the 20 nm Au film, which have been observed by scanning electron microscopy.