POS-NESY-13 Di, 23, 18:30 Gänge, Hochparterre, Rechts

Surface effects on the vibrational dynamics of glasses

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Glassy materials are characterized by a lack of short-range order which, however, does not inhibit the presence of phonon-like excitations. A highly debated topic in glass research are excess vibrational modes observed in neutron and Raman scattering spectra at energies where one would expect an $\propto \omega^2$ behavior in analogy with the Debye law for crystals. Such an excess, referred to as the boson peak, induces macroscopic "anomalies" at low temperatures (at about 1/10 of the Debye temperature) such as an excess of specific heat (still over the Debye expectations) and a plateau of the thermal conductivity where crystals exhibit a $\propto$ T3 dependence. Despite the intensive efforts which have been undertaken in the past in order to resolve the origin of these excess vibrational density of states, its nature is not fully understood. Recently, this fundamental phenomenon in the vibrational spectra of amorphous substances has been discovered as a surface effect by inelastic helium-atom scattering experiments [1,2].
Here we present measurements of the vibrational density of states of amorphous selenium by means of inelastic x-ray scattering in both bulk and surface-sensitive geometry, the latter is achieved by measuring at grazing incidence. First experiments from a liquid surface and a crystalline surface have been reported recently [3,4] and the theoretical framework for extracting a density of states from the coherent S(Q,ω) measurements has proven to give reliable results [5]. The experiment has been performed at the ID28 beamline of the ESRF exploiting the simultaneous availability of nine analyzers. While the surface effect seems to play no significant role on the boson peak, the gap which separates acoustic and optic modes in the bulk disappears at the surface. Surface-localized states are seen at 22 meV and preliminary model calculations for the amorphous Se surface indicate that these modes correspond to the optical phonon peak in the bulk density of states at 32 meV, however, shifted to lower energies due to the reduced forces acting on an atom situated at the surface.
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POS-NESY-14 Di, 23, 18:30 Gänge, Hochparterre, Rechts

Transformation of reverted austenite in a maraging steel under external load: an in-situ X-ray diffraction study using high-energy synchrotron radiation

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Reverted austenite strongly influences the mechanical properties of martensitic precipitation hardening steels (maraging steels). Therefore X-ray diffraction using high-energy synchrotron radiation was applied for in-situ studying the martensitic phase transformation under external load in a PH 13-8 Mo maraging steel. The volume fraction of austenite, the domain size of the crystallites, and the lattice parameters are obtained as function of strain for differently aged samples. It is shown that the reverted austenite is not mechanically stable under external load. A decrease of specific energy of transformation with increasing amount of initial austenite indicates a loss of stability of the austenitic phase with increasing aging time. Scanning of the fractured sample in longitudinal direction shows that the volume fraction of austenite and the domain sizes strongly depend on the distance from the point of fracture.

8.7 OGD – Oberflächen, Grenzflächen und dünne Schichten

POS-OGD-1 DI, 23, 18:30 Gänge, 2. Stock Links

The Interface of Sexiphenyl and Cu(110)

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We present an ab-initio density functional study on the electronic properties of a sexiphenyl (6P) monolayer adsorbed on the Cu(110) surface. 6P is a pi-conjugated, rod-like molecule consisting of a linear chain of six phenyl rings which is relevant for applications in organic light emitting diodes. Starting from the overlayer unit cell observed from low energy electron diffraction (LEED) we compute the adsorption geometry and the electronic structure of the interface which we compare to angle resolved photoemission data.

POS-OGD-2 Di,23, 18:30 Gänge, 2. Stock links

Cohesive and surface energies of organic molecular crystals

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First-principles calculations for the cohesive and surface energies of the oligoacene, oligophenylene and oligothiophene series are performed by density functional theory including non-local correlations to account for van der Waals interactions. Our work addresses the intermolecular bonding properties in these molecular crystals which are a prerequisite for understanding thin film growth and the resulting film morphologies. Our *ab-initio* results are in excellent agreement with available experimental data and represent a fundamental improvement over previous theoretical work relying on the local density approximation.

POS-OGD-3 DI, 23, 18:30 Gänge, 2.Stock Links