MM 28 Elektronische Eigenschaften

Zeit: Montag 10:30–12:00 Raum: TU H2038

MM 28.1 Mo 10:30 TU H2038

Surface Plasmon Resonance of Ag Nanotubes — •Yun Luo[1], Yixin Zhang[2], Martin Steinhart[1], Ralf B. Wehrspohn[3], Gunter Fischer[2] und Ulrich Gösele[1] — [1]Max-Planck-Institute of Microstructure Physics, Halle/Saale, Germany — [2]Max-Planck Research Unit for Enzymology of Protein Folding, Halle/Saale, Germamy — [3]Universität Paderborn, Warburger Strasse 100, Paderborn, Germany

Ag nanotubes and nanowires with outer diameters ranging from 25 nm to 400 nm and a shell thickness of 40 nm (in the case of tubes) have been fabricated via wetting of porous alumina templates and a subsequent annealing step at 350°C. Released nanotubes or nanowires with various diameters can be obtained by selectively removing the template.

In order to investigate the optical absorption properties of the 1D Ag nano-objects, they were dispersed in de-ionized water and placed in the beam path of a Hewlett-Packard Visible-ultraviolet spectrometer. During the measurement, the nanoobjects were kept suspended by stirring. The experimental absorption spectra carried out showed a sharp peak for Ag nanowires with a diameter of 25 nm at 374 nm. The peak position was shifted to longer wavelength and broadened when the diameter of the nanotubes was increasing.

FDTD calculations on both the transmission as well as the field distributions in the objects were performed assuming a dielectric constant corresponding to that of flat thin films. The calculated results show an agreement with the experiments curves

MM 28.2 Mo 10:45 TU H2038

Correlation-induced double-plasmon excitation in Al and Na — •C. Sternemann[1], S. Huotari[2], M. Volmer[1], G. Vanko[2], G. Monaco[2], M. Tolan[1], and W. Schülke[1] — [1]Institute of Physics, University of Dortmund, D-44221 Dortmund, Germany — [2]ESRF, BP 220, F-38043 Grenoble Cedex 9, France

Although the dynamic structure factor $S(\mathbf{q},\omega)$ of simple metals has been discussed extensively in terms of electron-ion interaction and electron-electron correlation, the separation of these two contributions in the analysis of $S(\mathbf{q},\omega)$ is not straightforward. In this study, a new type of structure in the $S(\mathbf{q},\omega)$ of simple metals was found. This structure originates solely from dynamic correlation effects in the homogeneous electron gas, and is not largely affected by electron-ion interaction.

The non-resonant inelastic x-ray scattering experiments have been performed at beamline ID16 of ESRF. The photon energy-loss spectra of both Al and Na have been measured for momentum-transfers between $0.7q_c$ and $1.5q_c$, i.e. across the plasmon cut-off vector q_c . For the first time, peaklike structures were found in the high-energy-loss tail of the dynamic structure factor of both metals. According to their shape, the q-dependence of their peak energies and intensities, these structures can be attributed to intrinsic plasmon-plasmon excitations, as proposed theoretically by Sturm and Gusarov [1]. Thus a new type of feature in S(q,w) has been observed which may give the opportunity to probe effects that are of second order in the dynamically screened Coulomb interaction.

[1] K. Sturm and A. Gusarov, Physical Review B **62**, 16474 (2000)

MM 28.3 Mo 11:00 TU H2038

Decoupling methods as dynamical mean field theory impurity solvers — •Harald Jeschke — Institut für theoretische Physik, Uni Frankfurt, Robert-Mayerstr. 8-10, 60054 Frankfurt/Main

The use of equation of motion decoupling methods as impurity solvers to be used in conjunction with the dynamical mean field self-consistency condition for the solution of lattice models is explored. By comparing the impurity solver to exact diagonalization results and applying it to lattice models like Hubbard model and Periodic Anderson model it is shown that the method could be a cheap alternative to computationally demanding methods like quantum Monte Carlo. The method works in a large range of parameters and promises to be useful in combination with density functional theory for the study of strongly correlated materials.

MM 28.4 Mo 11:15 TU H2038

Ab-initio Korrelationsrechnungen für V and Fe mit dem Lokalen Ansatz — •Gernot Stollhoff — Max Planck Institut f. Festkörperforschung, 70569 Stuttgart

Erstmals werden Resultate von ab-initio Korrelationsrechnungen mit dem Lokalen Ansatz für zwei Übergangsmetalle, nämlich V und (nichtmagnetisches) Fe präsentiert.

In beiden Fällen gibt es nennenswerte Abweichungen von den bekannten Dichtefunktionals (DF) - Resultaten. Bei V führen nicht lokale Austausch- und Korrelationsbeiträge zu einer Verschiebung der Fermiflächen und bringen sie in bessere Übereinstimmung mit dem Experiment. Bei Fe spielen diese Beiträge eine noch stärkere Rolle. Die Besetzungen in Hartree-Fock - und DF - Näherung unterscheiden sich gravierend. Die Besetzung des korrekten Grundzustandes liegt näher an der DF - Näherung, weicht aber deutlich ab. Entsprechend wird die Zustandsdichte modifiziert. Diese zeigt eine bessere Übereinstimmung mit den experimentellen Daten für Fe oberhalb des magnetischen Phasenüberganges.

MM 28.5 Mo 11:30 TU H2038

Al-TM(transition-metal) compounds: Non-isotropic electronic transport and bonding networks — •Torsten Schmidt and Heinrich Solbrig — Institute of Physics, Technical University of Chemnitz, D-09107

Alloys of these class, being similar to Si-based materials, cover a wide range of electronic properties between clearly metallic and even insulating. It has been shown experimentally[1] that covalent bonding is common in Al-TM systems.

A molecular-orbital analysis[2] reveals a strong bonding-antibonding splitting at next neighbors. We show that such bonds can combine to form extended bonding-networks which are covered by high valence density. Metallic systems of this kind have enhanced resistivities along directions which cross these bonding network.

We tread the above toppics in terms of a suitably defined network-bond-order by means of orbital based, as well as by scattering approaches.

[1] K. Kirihara *et al.* Phys. Rev. B68, 014205 (2003) [2] Krajčí and Hafner, J. Phys.: Condens. Matter 14, 5755 (2002)

MM 28.6 Mo 11:45 TU H2038

Redetermination and calculation of the thermopower of lead — •Horst Brodowsky and Matthias Albus — Institut f. Physikalische Chemie, Uni Kiel

Precise Thomson heat measurements by Roberts resulted in a shift of the previously accepted lead standard of Christian et al. by 0.30 μV/K. Superconductor measurements between 16 and 112 K suggest a shift of 0.41 ± 0.02 μV/K instead.

It has been shown for a number of transition metal alloys as well as for the alkali metals, that it is not necessary to calculate the ratio of the intractable transport coefficients of the Onsager equations. The diffusional thermopower happens to be equal to the more readily accessible entropy of the electrons divided by the electronic charge (Z. Metallkunde **90** (1999) 111; **91** (2000) 375; **93** (2002) 1164; **95** (2004) 698). This surprising result is obtained, because in metals the electron/atom ratio is constant along the length of the wire (besides the pressure) and the electrochemical potential of the electrons is a unique function of the temperature. This fact allows the more direct evaluation of Onsager's equation compared to the conventional method.