### Thursday, 05.09.2013, HS 5

| Time | ID | **SOFT MATTER AND OTHER SYSTEMS I**  
**SHARED WITH THE BIOPHYSICS SESSION**  
Chair: Georg Pabst, Uni Graz |
|------|----|---|
| 13:30 | 121 | Equilibrium and flow of cluster-forming complex fluids  
Christos N. Likos (i) |
| 14:00 | 122 | Optimized Fourier Monte Carlo Simulation of Solid and Hexatic Membranes  
Andreas Troester |
| 14:15 | 123 | Biomimetic folding particle chains  
Peter Oostrom |

**SOFT MATTER AND OTHER SYSTEMS II**  
Chair: Oskar Paris, Uni Leoben |
| 14:30 | 124 | Small Angle Scattering Study of the self-assembly of an amphiphilic designer peptide from the monomer to a helical superstructure  
Heinz Amenitsch |
| 14:45 | 125 | Liquid Structure and the Noncoincidence Effect of Liquid Dimethyl Sulfoxide Revisited  
Maurizio Musso |
| 15:00 | 126 | Generation of multiply twinned Ag clusters (n<6000) in superfluid helium nanodroplets  
Philipp Thaler |
| 15:15 | 127 | The characterization of defects in silicon by Electron Beam Induced Current (EBIC) measurements  
Peter Hadley |
| 15:30 | | **Coffee Break** |

**SEMICONDUCTORS**  
Chair: Peter Hadley, TU Graz |
| 16:00 | 131 | Structural Investigation of Novel Semiconductor Systems by Transmission Electron Microscopy  
Heiko Groiss (i) |
| 16:30 | 132 | Harnessing nuclear spin polarization fluctuations in a semiconductor nanowire  
Phani Peddibhotla |
| 16:45 | 133 | Structural and magnetic properties of ZnO with doping beyond the coalescence limit  
Verena Ney |
| 17:00 | 134 | μ-Raman investigation of heterogeneously strained Si nanostructures  
Martin Süess |
| 17:15 | 135 | Normally-off GaN MOSHEMTs with thin barrier on Si substrate  
Alexander Alexewicz |
| 17:30 | 136 | Spin dependent electron response functions  
Raphael Hobiger |
| 17:45 | 137 | Creation and detection of entanglement in helical edge states using a single-electron source  
Patrick Hofer |
| 18:00 | 138 | Experimental observation of the even-denominator fractional quantum-Hall effect in suspended graphene bilayers  
DongKeun Ki |
| 18:15 | 139 | Magneto-optical spectroscopy of epitaxial graphene  
Iris Crassee (talk given by Alexey Kuzmenko) |
| 18:30 | | **Postersession and Apéro** |
| 20:00 | | **Conference Dinner** |

### Friday, 06.09.2013, HS 5

| Time | ID | **CONDENSED MATTER COMPUTATIONAL AND THEORY**  
Chair: Christian Rüegg, PSI Villigen & Uni Genf |
|------|----|---|
| 13:30 | 141 | Computer simulations of strongly correlated quantum matter  
Andreas Läuchli (i) |
| 14:00 | 142 | A variational cluster approach to strongly correlated quantum systems out of equilibrium  
Martin Nuss |
| 14:15 | 143 | Exotic Bound States in Low Dimensions  
Jelena Klinovaja |
| 14:45 | 144 | Berry Phase Effect in Solids  
Gerhard Brunthaler |
| 15:00 | 145 | First-principle investigation of topological transition in α-Sn nanocrystals  
Sebastian Küfner |
| 15:15 | 146 | A modified Griffith model for explaining Liquid Metal Embrittlement in the Fe/Zn system  
Klaus-Dieter Bauer |
| 15:30 | | **END** |

**ID**

| 151 | Conduction and Valence Band States of Sb-Mediated Ge Quantum Dots in n-type Si Studied by Deep Level Transient Spectroscopy  
Victor Tapio Rangel Kuoppa |
| 152 | Ultra-small-angle polarised neutron scattering on magnetic structures  
Erwin Jerich |
| 153 | Low temperature magnetic structure of multiferroic YBaCuFeO_{5}  
Mickael Morin |
| 154 | Dynamic stabilization of nonequilibrium domain configurations in magnetic squares with high amplitude excitations  
Stephanie Stevenson |
| 155 | Parametric polariton scattering in coupled planar microcavities  
Patrick Mai |
| 156 | Magnetism on the route of compensated to remnant magnetism: SQUID- and Raman-data on NiO-nanoparticles  
Julia Weber |
| 157 | Skyrmion Dynamics in Perpendicular Magnetic Anisotropy Nanostructures  
Christoforos Moutafis |
| 158 | Neutron diffraction study of lattice damage induced by tritium decay in palladium tritide  
Gerhard Krexner |
| 159 | Effects of Geometrical Confinement on Li and Na in Nanoporous Glasses  
Gerhard Krexner |
| 160 | SiGe self-assembled nanostructures: from surface science to quantum transport  
Georgios Katsaros |
| 161 | Enhanced 1.54 μm-Er^{3+} photoluminescence through contact coupling with Ge nanostructures  
J. Martin-Sánchez |
| 162 | Refinement of the eutectoid region of the Fe-Ru phase diagram using thermodynamic and metallurgical approaches  
Gabriela Schimo |
| 163 | Conducting Cellulose Fiber Networks as Flexible Substrate for Optoelectronic Applications  
Bettina Friedel |
First-principle investigation of topological transition in a-Sn nanocrystals

Sebastian Küfner, Lars Matthes, Jürgen Furthmüller, Friedhelm Bechstedt
FSU Jena, Max-Wien Platz 1, DE-07743 Jena

We use density-functional theory within local XC-functionals to show that the level-ordering of s- and p-like states at Gamma in α-Sn nanocrystals is inverted with respect to the bulk. Showing that the fundamental energy gap decreases for increased nanodot-diameter, we conclude the occurrence of a topological transition for a certain diameter where the level ordering changes. As an important ingredient spin-orbit interaction is taken into account. In addition, we prove that our results concerning the fundamental energy gaps of the nanocrystals agree perfectly with results obtained by methods considering many-body effects and screened coulomb-interaction.

A modified Griffith model for explaining Liquid Metal Embrittlement in the Fe/Zn system

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1 Zentrum für Oberflächen- und Nanoanalytik, Johannes Kepler Universität Linz, Altenberger Str. 69, AT-4040 Linz
2 Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, DE-40237 Düsseldorf

In the manufacturing of high quality steel products processing time and cost can be reduced by hot-forming previously coated steel sheets. For galvanized steel sheets, however, a degradation of workpiece quality is observed caused by Liquid Metal Embrittlement (LME) in the presence of liquid zinc. We performed density functional theory simulations of [111] and [110] tilt grain boundaries of bcc iron (ferrite) and applied the adapted Griffith model described by Nicholas and Old (1979). This predicted spontaneous failure in the absence of strain, contradicting experimental findings at voestalpine AG. A modification of the model allowed us to bridge the gap between theory and experiment.

Conduction and Valence Band States of Sb-Mediated Ge Quantum Dots in n-type Si Studied by Deep Level Transient Spectroscopy

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2 Max Planck Institute of Microstructure Physics, Weinberg 2, DE-06120 Halle

Deep level transient spectroscopy technique is used on a Ti Schottky diode on n-type silicon with embedded Sb-mediated Ge quantum dots (QDs). We discovered an electron trap and two hole traps within the Si band gap at the plane of Ge QDs. An electron trap has activation energy of 87±7 meV. One hole trap has activation energy of 304±32 meV, while the second hole trap is represented by the energy sub-band between 125 and 250 meV above the top of the Si valence band. The electron level (87±7 meV) and the hole energy sub-band (125-250 meV) are identified as energetic states of Ge QDs array. The deepest trap level for holes (304 meV) has not been identified yet.

Ultra-small-angle polarised neutron scattering on magnetic structures

Erwin Jericha, Christoph Gösselsberger, Wielfried Mach, Tobias Rechberger, Alexander Zdarzil, Gerald Badurek, TU Wien, Atominstitut, Stadionallee 2, AT-1020 Wien

Ultra-small-angle scattering of polarised neutrons (USANSPOL) allows for the study of magnetic microstructure. The technique takes advantage from the narrow angular width of the Bragg reflection by perfect crystals, and polarisation of the neutron beam is obtained by magnetic prism. Scattering of spin-up and spin-down neutrons is recorded in a single measurement and identified by an angular shift of their respective scattering curves. We present new results on magnetic ribbons which are illustrative examples for developing the USANSPOL technique. These measurements allow an assessment of the evolution of magnetic structure under the influence of external magnetic fields and mechanical stress.