

HL 29: New materials

Time: Tuesday 12:00–13:15

Location: ER 164

HL 29.1 Tue 12:00 ER 164

Heusler compounds as thermoelectric materials — ●JOACHIM BARTH¹, BENJAMIN BALKE¹, FRED CASPER¹, GERHARD H. FECHER¹, JUERGEN WINTERLIK¹, CLAUDIA FELSER¹, ROSA ROBERTS², ANDRE SHKABKO², and ANKE WEIDENKAFF² — ¹Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz — ²Empa - Materials Science and Technology, Ueberlandstrasse 129, CH-8600 Duebendorf

Thermoelectric materials have gathered a lot of interest in the recent years. They can be either used in power generating devices or in heating and cooling systems. Several materials show interesting properties; among them are the Heusler and Half-Heusler compounds. These material classes are of special interest because they are very diverse and can be easily tuned to the needs of applications. To illustrate the diversity and tunability of these materials several compounds and the creating process are presented.

The process of finding promising materials includes three steps. At first we use band structure calculations to identify promising compounds. In the second step we synthesize them by arc melting, which is followed by annealing. During the final step we characterize them by measuring XRD, electrical and thermal conductivity and Seebeck coefficient. The quality of the compounds as thermoelectric materials is determined by the Power Factor and the Figure of merit.

HL 29.2 Tue 12:15 ER 164

Orientational ordering and intermolecular interactions in the rotor-stator compounds C₆₀-C₈H₈ and C₇₀-C₈H₈ under pressure — ●KOMALAVALLI THIRUNAVUKKARASU¹, CHRISTINE A. KUNTSCHER¹, GYULA BÉNYEI², ISTVÁN JALSOVSZKY², GYÖNGYI KLUPP³, KATALIN KAMARÁS³, ÉVA KOVÁTS³, and SÁNDOR PEKKER³ — ¹Experimentalphysik II, Universität Augsburg, D-86159 Augsburg, Germany — ²Department of Organic Chemistry, Eötvös Loránd University, P.O.Box 32, Budapest, Hungary H 1518 — ³Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, P.O.Box 49, Budapest, Hungary H 1525

The fullerene-cubane molecular crystals C₆₀-C₈H₈ and C₇₀-C₈H₈ are the first members of the rotor-stator crystal family [1]. Static C₈H₈ molecules occupy the octahedral voids of the fullerene fcc structure and act as bearings for the rotating fullerene molecules. On cooling, C₆₀-C₈H₈ undergoes a phase transition at 140 K due to orientational ordering of the C₆₀ molecules, while C₇₀-C₈H₈ undergoes transitions at around 390 K and 150 K. A first pressure-dependent transmittance study revealed an orientational ordering transition in C₆₀-C₈H₈ induced at 0.8 GPa [2]. We have extended our spectroscopic studies to a broad frequency range for both C₆₀-C₈H₈ and C₇₀-C₈H₈ to monitor the vibrational properties and the absorption edge as a function of pressure. The nature of the observed anomalies and the electronic properties under pressure will be discussed. *Supported by the DFG.* [1] S. Pekker et al., *Nature Materials* **4**, 764 (2005). [2] C. A. Kuntscher et al., *Phys. Stat. Sol. (b)* **243**, 2981 (2006).

HL 29.3 Tue 12:30 ER 164

Numerical simulation of a fractal meta structure in the microwave regime — ●ERNST LENZ, BENJAMIN MEIER, and HEINO HENKE — TU Berlin, Fachgebiet Theoretische Elektrotechnik EN-2, Einsteinufer 17, 10587 Berlin, Germany

Metamaterials are artificial structures with novel and promising properties [1,2,3,4]. To reduce the unwanted scattering and diffraction effects of incoming electromagnetic waves it is necessary to achieve a higher degree of homogenization [1]. Therefore usually the unit cell size d is varied, while the wavelength λ remains constant.

We present simulation results of a fractal meta structure where we have replaced the well known split ring resonator (SRR) [2,3] by two

concentric Koch snowflakes [5]. In that way a remarkable reduction of the resonance frequency could be achieved as compared to the SRR structure of the same spatial extent. Furthermore this results in a higher degree of homogenization of the introduced meta structure. Additionally we show that left-handed behavior is supported by simulation results as well as obtained by experimental data.

[1] V. G. Veselago, *Sov. Phys. Usp.* **10**, 509 (1968). [2] J. B. Pendry et al., *IEEE-TMTT* **47**, 2075 (1999). [3] D. R. Smith et al., *PRL* **84**, 4184 (2000). [4] N. Engheta et al., *IEEE-TMTT* **53**, 1535 (2005). [5] K. J. Falconer, *Fraktale Geometrie*, Spektrum, Berlin (1990).

HL 29.4 Tue 12:45 ER 164

Beaded carbon nanofilament via chemical vapor deposition — ●LI SONG¹, ALEXANDER W. HOLLEITNER², HUIHONG QIAN³, ACHIM HARTSCHUH³, EVA M. WEIG¹, and JÖRG P. KOTTHAUS¹ — ¹CeNS und Fakultät für Physik, Ludwig-Maximilians-Universität, 80539 München — ²Walter Schottky Institut, Technische Universität München, 85748 München — ³Department für Chemie, Physikalische Chemie, Butenandtstr. 5-13, 81377 München

Due to their low density and extraordinary mechanical properties, carbon filaments and fibers have large commercial applications as reinforcements in composite materials. In order to transfer the maximum load onto the filaments, the interfacial strength between the host matrices and the filaments should be as high as possible. The interfacial strength mostly depends on the surfaces and shapes of the reinforcing filaments. Here, we present a chemical vapor deposition method to synthesize carbon nanofilaments with carbon beads on their surface. The stems of the nanofilaments typically show an average diameter of about 60 nm, while the diameter of the beads is in the range of 200-400 nm. By SEM and AFM analysis we find a necklace-like structure of the carbon nanofilaments. Raman spectra reveal that the beads are made of graphite, while the stems are multi-walled carbon nanotubes admixed with graphite and carbon fibers. The beaded carbon nanofilaments may have applications as reinforcing agents because the mechanical interlocking between beads can produce stronger interfacial adhesion.

HL 29.5 Tue 13:00 ER 164

AVD and ALD developments for next generation MIM capacitors and memory applications — PETER K. BAUMANN, CHRISTOPH LOHE, and ●MICHAEL HEUKEN — AIXTRON AG, Aachen, Germany

Atomic layer deposition (ALD) enables deposition of electrode, dielectric and barrier layers on high aspect ratio trench structures and has been widely used. However, due to its nature the throughput is typically limited. Atomic vapor deposition (AVD[®]) is a special type of metal organic vapor deposition (MOCVD) that enables deposition with high precursor gas phase saturation. This results in improved throughput while maintaining conformal deposition on moderate aspect ratio trench structures. Based on the International Roadmap for Semiconductors (ITRS) for front end, for DRAM at the 50nm and below technology node metal-insulator-metal (MIM) structures will be required [1]. Also conformal step coverage on structures with aspect ratios of 1:60 and higher as well as an equivalent oxide thickness (EOT) of less than 1nm will be necessary. Other memory applications (e.g. phase change memory) require less advanced aspect ratios, opening possibilities for AVD[®]. ALD and AVD[®] have been used to deposit electrode and dielectric films based on e.g. TiN, Ru, TaSiN as well as HfO₂, ZrO₂, Al₂O₃. Results for the different deposition techniques and various process conditions will be presented and compared considering use for memory applications.

[1] Front end, International Roadmap for Semiconductors (Semiconductor Industry Association, Palo Alto 2006 update).