

FA2-MS14-P01

Correlation of structure and conductance in nanowires. Sibylle Gemming. *Institute of Ion Beam Physics and Materials Research, FZ Dresden-Rossendorf, P.O. Box 51 01 19, D-01314 Dresden, Germany.*
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In nanostructured materials spatial confinement effects lead to structure-dependent deviations from the bulk transport properties. Such modifications may in part be accounted for by classical transport simulations, but a microscopically more detailed and mostly parameter-free picture is obtained from quantum-mechanical density-functional theory (DFT).

DFT calculations yield the atom arrangement and electronic structure of nanotubes and nanowires in the electronic ground state. Additionally, an extension by a Green's function formalism leads to the determination and analysis of electronic transport through contacted nanostructures. A combination of both approaches allows correlating structural and transport properties of nanostructures. The applicability of this approach will be demonstrated for mechanically triggered changes of the conductivity [1] up to the metal-insulator transition [2, 3] in nanowires.

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Keywords: nanostructures, density-functional theory, electromechanics

FA2-MS14-P02

Long-range order and thermal stability of thin Co₂FeSi films on GaAs. Bernd Jenichen^a, Jens Herfort^a, Kazuhide Kumakura^{a,b}, Thomas Hentschel^a, Achim Trampert^a. ^a*Paul-Drude-Institut, Berlin, Germany.* ^b*NTT Basic Research Laboratories, Atsugi-shi, Kanagawa, Japan.*
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Co₂FeSi is a ferromagnetic half-metal with a Curie temperature larger than 1100 K. The lattice parameter matches that of GaAs. Therefore, Co₂FeSi is suitable for spin injection into GaAs-based structures such as spin light-emitting diodes [1]. Co₂FeSi/GaAs hybrid structures are grown by molecular beam epitaxy [2] and characterized by x-ray (XRD) and electron diffraction, transmission electron microscopy (TEM), atomic force microscopy, and secondary ion mass spectrometry. Films grown on GaAs(111)B have a stable interface up to a growth temperature $T_s = 275^\circ\text{C}$, which is 75 K higher than the temperature guaranteeing a stable interface during growth on GaAs(001) and GaAs(110). Despite the vanishing lattice misfit between the Co₂FeSi film and the GaAs buffer layer, we found a typical grain structure of the film (see e.g. TEM micrograph in the Figure), which is strong evidence for three-dimensional island growth during the stage of heteroepitaxy before a continuous film is formed [3,4]. Nevertheless the heteroepitaxial hybrid-structures are free of dislocations. The films contain the fully ordered $L2_1$ and the partially ordered $B2$ phases. Long-range order of the Co₂FeSi lattice improves with increasing T_s . However, near the Co₂FeSi/GaAs interface we often find (by combined XRD and TEM analysis) some disordering ($B2$ phase). The spatial distribution of long-range order in the films is imaged using a comparison of superlattice and the corresponding fundamental

reflections. Order parameters, i.e. the fraction of Si atoms occupying Fe and Co sublattices are determined. Spatial inhomogeneities of longrange order can be explained by local non-stoichiometry.

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On the structure of a geopolymer binder. Elzbieta M. Mielcarek, Claus H. Rüscher. *Institute for Mineralogy, Leibniz University of Hannover, Germany.*
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The binding properties of aluminosilicate gels were considered for more than 40 years under the name "Geopolymer" [1]. Herein the mechanical strength has been explained with the growth of an aluminosilicate network enforced e.g. by alkali activation of metakaolin (MK) using waterglass (WG) solution, seen as the basic system for studying "geopolymerisation". However, the structure of the binder phase has not well been understood as was also stressed in the most recent review in this field [2]. New insights on geopolymerisation could be based on molybdate, Raman and infrared spectroscopic methods in combination with mechanical strength measurements [3, 4]. It could be shown that the mechanical strength increases mainly because the slowly forming aluminosilicate network encloses preformed polysilicate chain units (more than 30 Si-O units long). These chain units are formed due to the extraction of hydroxide from the waterglass in the dissolution of metakaolin, a fact which has to some surprise been overlooked in previous studies. We show here that an optimal reacted binder phase is observed for effective ratios of Si/Al = 2 and K/Al = 1 related to a certain WG/MK ratio. Decreasing the WG/MK ratio produces always about the same binder phase but lead to a significant portion of unreacted metakaolin, as shown by infrared absorption spectroscopy and X-ray diffraction method. The concentration of binder phase and undissolved material are responsible for hardening and weakening process of geopolymer. The systematic structural variation over time followed by IR and Thermogravimetric method (TG, DTA) demonstrated close relation between the extend of water evaporation and condensation degree of binder phase. It is concluded that during heating process condensation of aluminosilicate network and partially decomposition of silicate chains occurs depending on pre-aging time of the sample.

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