Growth and characterization of one-dimensional semiconductor nanocrystals within single-walled carbon nanotube channels

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One-dimensional (1D) crystals of compound semiconductors with a diameter of 3-5 atoms currently attract attention due to their unique properties, in particular size-dependent quantum effects like van Hove singularities etc. [1]. From the fundamental perspective, it is also of importance to understand the interplay between the electronic and atomic structure of the 1D-crystals and the relationship between the structural parameters of a 1D-crystal and the bulk. Unfortunately, in practice it is difficult to prepare and study 1D-crystals in its free state. Within the last decade it has been proposed to use single-walled carbon nanotubes (SWCNTs) as a template for growing 1D-crystals since these nanotubes are known to be chemically inert towards moSt inorganic substances; under certain conditions, it is also possible to avoid a charge transfer between the crystal and the nanotube wall [2].

The aims of this work were the synthesis of SnTe 1D crystals in channels of SWCNTs with inner diameter 1-1.4 nm and characterization of the atomic structure and the crystal-template interactions for SnTe@SWCNT nanocomposite. The synthetic strategy was based on the impregnation of pre-opened single-walled carbon nanotubes by molten salt in vacuum.

TEM measurements in combination with DFT calculations clearly show that the atomic structure of the 1D SnTe crystals corresponds to $(SnTe)_{5n}$ with a significant bond lengths relaxation (contraction) along the SWCNT axis in comparison to the bulk structure. The effective charges of both the Sn and Te atoms are lower than in the bulk of SnTe. X-ray photoemission and Raman spectroscopy data show no noticeable interaction between the 1D SnTe crystal and the SWCNTs, except for a minor influence of the intercalated crystal on metallic SWCNTs. From this observation we conclude that the reported relaxation effects for the bond lengths are inherent to the 1D SnTe crystal. This also suggests that SnTe@SWCNT is a well-suited model system to study the physics of non-interacting 1D-crystals.

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