Contribution ID: **106** Type: **Oral contribution**

Crystal structure and lattice dynamics of endotaxial $FeSi_2$ nanowires

Tuesday 16 March 2021 16:15 (20 minutes)

Metallic silicides constitute an important part of current microelectronics, serving as Schottky barriers and ohmic contacts, gate electrodes, local interconnects, and diffusion barriers [1–3]. Silicide nanowires, self-organized on the Si(110) surface, are considered as building blocks of future nanoelectronics and have been intensively investigated [4]. However, the reports about their crystal structure remain contradictory, spanning cubic (s or γ) [5–7] and tetragonal (α) [8] phases. Furthermore, in nanostructures the lattice vibrational waves (phonons) deviate drastically from those in bulk crystals, giving rise to anomalies in thermodynamic, elastic, electronic, and magnetic properties. Hence, a thorough understanding of the physical properties of these materials requires a comprehensive investigation of the crystal structure and lattice dynamics as a function of the nanowire size.

Using extended x-ray absorption fine structure (EXAFS) spectroscopy and nuclear inelastic scattering (NIS) we performed a systematic study of the crystal structure and the lattice dynamics of endotaxial $FeSi_2$ nanowires, which are in-plane embedded into the Si(110) surface. The EXAFS results unveiled the formation of the metastable, surface-stabilized α phase. The Fe-partial phonon density of states, obtained by the NIS experiment, exhibits a broadening of the spectral features with decreasing nanowire width and a pronounced vibrational anisotropy that originates from the specific orientation of the tetragonal α–$FeSi_2$ unit cell on the Si(110) surface. The results from first-principles calculations are fully consistent with the experimental observations [9].

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Session Classification: Micro and nano-crystalline materials

Track Classification: Micro and nano-crystalline materials