Vibrational Properties of Nanograins and Interfaces in Nanocrystalline Materials

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Vibrational Properties of Nanograins and Interfaces in Nanocrystalline Materials

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The vibrational dynamics of nanocrystalline $Fe_{90}Zr_7B_3$ was studied at various phases of crystallization by ^{57}Fe nuclear inelastic scattering of synchrotron radiation. The average sizes of the nanograins were determined by the Rietveld refinement of the X-ray diffractograms, while the volume fraction of the interfaces was obtained from the conversion electron Mössbauer spectra by applying a well established fitting model [1, 2]. The density of phonon states (DOS) of the nanograins was separated from the DOS of the interfaces for a wide range of grain sizes and interface thicknesses. Surprisingly, DOS of the interior and the surface of the nanograins do not vary with the grain size and closely resembles that of the bulk material down to 2 nm. The anomalous enhancement of the phonon states at low and high energies observed in the DOS of the nanocrystalline materials [3], originates entirely from the vibrational modes of the interface exhibiting a characteristic DOS of a significantly disordered matter. The low energy enhancement of phonon states scales linearly to the volume fraction of the interfaces and perfectly obeys the Debye law for the interface thickness below 0.5 nm.

The obtained results give an unambiguous evidence that the anomalous dynamics and thermodynamics of nanocrystalline solids originate from the disordered interfaces, while thermodynamical properties of the nanograins are essentially bulklike and to a large extent size-independent. These findings are of significant importance for the continuously increasing number of technological applications of the nanocrystalline materials. In particular they reveal that tailoring of certain thermo-elastic properties requires to control precisely the volume fraction of the nanograins rather than of their sizes.

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