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Vibrational thermodynamics of nanocrystalline materials

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Abstract:

The vibrational thermodynamics of nano-scale materials has attracted a lot of attention due to the observed striking differences of their atomic vibrations relative to the bulk counterparts [1]. The observed anomalies are the enhancement of their density of phonon states (DOS) at low and high energies and broadening of the phonon peaks. In addition, the energy dependence of the low-energy part of their DOS has been a source of long-standing debates. The experimental and theoretical results are contradictory reporting linear, power low, and Debye-like behavior.

In order to further clarify this issue we have studied the vibrational properties of a nanocrystalline Fe90Zr7B3 alloy prepared by crystallization of an amorphous precursor. The atomic vibrations of the nanograins were separated from those of the interfaces for a wide range of grain sizes and interface thicknesses. Surprisingly, the results show that the atomic vibrations of the nanograins do not vary with their size and even down to 2 nm closely resemble those of the bulk [2]. The observed anomalies of the vibrational and thermodynamic properties originate solely form the atoms located at the nanocrystalline interfaces [3].

[1] B. Fultz , Prog. Mater. Sci. 55, 247 (2010).
[2] S. Stankov et al., PRL 100, 235503 (2008).
[3] S. Stankov et al., PRB 82, 144301 (2010).