Atomic Dynamics at the Nano Scale

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The dynamics of nano-scale materials has attracted a lot of attention during the last years due to the observed striking differences of their atomic vibrations relative to the bulk counterparts. The observed anomalies are the enhancement of their density of phonon states (DOS) at low and high energies and broadening of the phonon peaks [1-4]. In addition, the energy dependence of the low-energy part of their DOS has been a source of long-standing debates. The experimental results are contradictory reporting a linear dependence [5], a power low with n=1.33 [6], and a Debye behavior [1-4]. On the other hand the theoretical calculations has also indicated that non-Debye dynamics could originate from the atoms located at the surfaces [7], at the grain boundaries [8], or in the porous areas [9] of the nanocrystalline (NC) materials. In order to find a consistent picture of the atomic dynamics at the nano scale one has to precisely disentangle the effects of disorder, chemical state, and reduced dimensionality.
A recent instrumentation development [10] at the Nuclear Resonance beamline of the ESRF has allowed for a precise study of the atomic vibrations at and near a clean (110)Fe surface [11]. The thickness evolution of the phonon DOS of ultrathin Fe films has also been studied [12]. Both experiments revealed a Debye-like enhancement of the phonon states at low energy originating from surface-specific modes, also confirmed by the theory.
However, it is not very likely that such surface phonon modes are responsible for the observed anomalies in the DOS of bulk NC materials where clean and well-ordered surfaces can not be found. In order to further clarify this issue we have studied the vibrational properties of a NC $Fe_{90}Zr_7B_3$ alloy prepared by crystallization of an amorphous precursor. The data analysis have shown that the known anomalous features originate solely from the disordered interfaces, while the DOS of the nanograins are bulk-like and size-independent [13].

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