**Vibrational properties of nanoparticles: finite size and oxidation effects**

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The investigation of vibrational dynamics in low-dimensional and nanostructured solids is a rapidly growing research field, powered by the interest in thermodynamic, conductive, and optical properties of mesoscopic systems [1]. In the vibrational density of states (VDOS, $g(E)$) of nanocrystalline (NC) materials, both finite-size effects and interface-related phenomena due to the large fraction of disordered interfaces are expected. In particular, two basic questions are extremely relevant: (i) how does the VDOS scale with the crystallite size $d$, and (ii) is there a deviation from the usual Debye law $g(E)=aE^2$ at low energies ? Nuclear inelastic scattering (NIS) of synchrotron radiation was employed to determine the VDOS in NC Fe samples with different $d$, prepared by gas-phase condensation [2]. NIS experiments were carried out on ID18 at ESRF, with a final bandwidth of 0.6 meV.

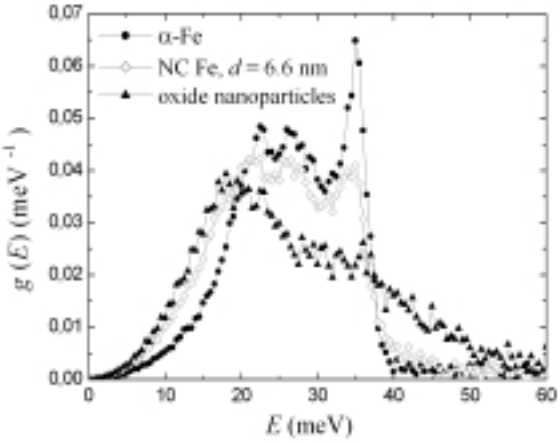


Figure 1 VDOS of NC iron ($d$=6.6 nm), iron oxide nanoparticles, and reference α-Fe.

In NC samples, in comparison with a reference α-Fe foil, an enhanced population of low-energy modes and a broadening of the longitudinal peak at about 36 meV is observed (Figure 1) [2]. This softening is due partly to oxidation and partly to vibrations of atoms at the crystallite interfaces, with modified local environment and softened force constants. The low-energy VDOS exhibits a $g(E)=aE^2$ dependence over the whole range 1.5-15 meV, and the coefficient $a$ increases with decreasing $d$. The broadening of the longitudinal peak is attributed to damping of phonons in confined geometry. The damping parameter Γ, determined from a convolution procedure [2], varies from 1.1 to 0.5 meV when $d$ passes from 6.6 to 13 nm. The $d$-dependence of the parameter Γ indicates that phonon lifetime $\tau \approx 2\hbar/\Gamma$ and mean free path λ decrease with decreasing $d$. For $d$=6.6 nm, it is estimated that λ≈3 nm.

**References**

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