Phonons at the Fe(110) surface

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We studied atomic vibrations of a clean Fe (110) surface. The samples were prepared, characterized, and measured *in situ* in ultra-high vacuum conditions. The density of phonon states $g(E)$ was measured separately for the first, second, and further atomic monolayers using nuclear inelastic scattering of synchrotron radiation.

The results show that atoms of the first layer vibrate with frequencies significantly lower and amplitudes much larger than those in the bulk. Furthermore, the surface atoms reveal a remarkable difference in vibrational spectra along two perpendicular in-surface directions. These vibrational anomalies are localized strictly on the surface, i.e., the vibrations of the second monolayer are already very close to those of the bulk. The softening of vibrations does not change the Debye-like behavior $g(E) \propto E^2$ of the DOS at low energies.

The experimental observations are in excellent agreement with the first principles calculations. Strong enhancement of the surface DOS at low frequencies arises from the surface phonon modes and from an overall softening due to missing neighbors. The broken translational symmetry along the surface normal is reflected as in plane anisotropy of elastic properties.