Phonons of surfaces and nanostructures

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The aim of my talk is to present an overview of theoretical studies of the vibrational dynamics and thermodynamics of a set of nanostructured surfaces, nanoparticles, and other surface nanostructures. These include surfaces with regularly spaced steps and kinks (chiral surfaces) of varying local geometry and terrace width, and nanoparticles with single and multigrains as well as alloy nanoparticles. From these broad and extensive studies, two distinguishing features emerge from the results obtained for this set of systems with under coordinated atoms in diverse geometrical environments. The calculated phonons spectra show a systematic enhancement of modes at the lower end of the frequency spectrum and characteristic modes appear above the top of the bulk band. The origin of these novel features and their influence on the local vibrational entropy contributions are discussed. The unified behavior in the dynamical properties of these nanoscale materials may be rationalized in terms of the local coordination in these systems in which the constituent fcc metals display a correlation between the bond-length and bond-order.

However, our recent studies of the structure and vibrational dynamics of alloy nanoparticles show that the coordination alone is not enough to explain the novelty of the results. I will show in details when nano-alloys resemble their single element counterparts and when they differ.