Lattice dynamics of iron-based superconductors and related compounds

M. Opacic[1], N. Lazarevic[1], D. Tanaskovic[2], C. Petrovic[3] and Z.V.Popovic[1,4]
[1]*Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, Serbia*
[2]*Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade University of Belgrade, Serbia*
[3]*Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, New York, USA*
[4]*Serbian Academy of Sciences and Arts, Belgrade, Serbia*
e-mail: marko.opacic@ipb.ac.rs

The lecture focuses on vibrational properties of some unconventional iron-based superconductors and related compounds by means of Raman spectroscopy. In the measured phonon spectra of superconducting $K_xFe_{2-y}Se_2$ and nonsuperconducting $K_{0.8}Fe_{1.8}Co_{0.2}Se_2$ single crystals there are phonon modes originating from metallic/superconducting *I4/mmm* phase and insulating *I4/m* phase with ordered Fe vacancies. Temperature analysis of energy and linewidth of the vibrational modes were done using the model which takes into account lattice thermal expansion and anharmonic effects. The modes originating from the *I4/m* phase are well described by that model. On the other hand, A_{1g} mode energy in the superconducting sample exhibits sudden jump, which was ascribed to the change in the electronic structure when entering the superconducting state. By investigating Raman spectra of $K_xFe_{2-y}Se_2$ single crystals doped with various Co concentrations, the evolution of phase separation was followed. With increasing cobalt content phonon modes from the *I4/m* phase disappear and in Raman spectra remain only two phonon modes originating from the high symmetry *I4/mmm* phase. Broad asymmetric structure in the samples with intermediate Co concentrations was interpreted as a fingerprint of strong crystalline disorder. The presence of only two phonon modes in the end member of this sequence - $K_xCo_{2-y}Se_2$ - excludes the possibility of ordered vacancies. Measured Raman spectra show that ferromagnetic phase transition around 74 K in this single crystal has significant impact on phonon mode behavior. Namely, above the ferromagnetic transition, temperature dependence of phonon energy and linewidth looks conventional. On the other hand, below critical temperature both modes exhibit sudden hardening, A_{1g} mode narrows and B_{1g} one significantly broadens, which is ascribed to the spin-phonon and electron-phonon interaction. Large linewidth of the Raman modes originates from the electron-phonon coupling enhanced by the crystal disorder and spin fluctuation effects.