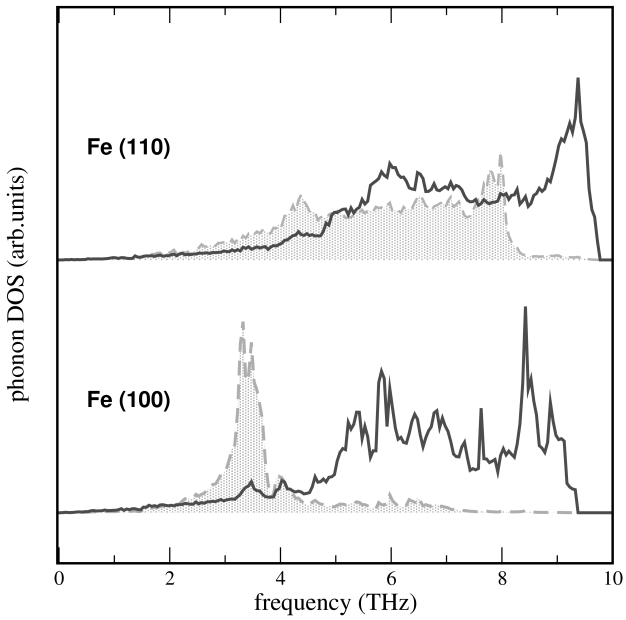
# *Ab initio* study of vibrational properties of iron (100) and (110) surfaces

Jan Łażewski
*Institute of Nuclear Physics Polish Academy of Sciences,*
*Radzikowskiego 152, 31--342 Kraków, Poland*

Simulation of iron surfaces, careful analysis of their structural and dynamical properties as well as electronic and magnetic structures should be a helpful step to better understanding of iron mono-layer properties. Therefore the first-principles calculations based on spin-polarized density functional theory (DFT) have been performed for two different iron slabs including (100) and (110) surfaces. For both systems lattice parameters and magnetic moments have been analyzed as a function of slab layers. Based on force constants direct method phonon dispersion relations and phonon density spectra have been calculated.




Calculated total phonon densities of states. Dashed lines depicted *xy*-surface contribution and solid lines *xy* phonon states for internal layer

Similarities and differences of both systems will be presented. In particular a significant difference between surface phonon states distribution will be discussed.

This work was partially supported by European Community under FP6 contract No. NMP4-CT-2003-001516 (DYNASYNC).