

# Spin-spiral Dispersion And Magnon-phonon Interactions In FCC-Fe

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Unlike BCC-Fe, some theoretical studies show that FCC-Fe is a weak magnet exhibiting magnetovolume instability and non collinear magnetic structure under compression. We did calculations for volume dependence of spin-spiral dispersion in FCC-Fe, the approach implemented in the Vienna Ab initio Simulation Package (VASP). It is shown that at low volumes, the magnetic configuration corresponding to the ground state is a spin-spiral at  $q_2=2\pi/a(0.2,0,1)$ , whereas for higher volumes the ground state is at  $q_1=2\pi/a(0,0,0.6)$ . We found VASP package is a reliable tool for the calculation of spin-spiral structure because almost all the results we got are consistent with the data from full-potential linearized augmented-plane-wave method (FP-APW+lo) study<sup>1</sup>. Besides that, such system may also show some structural instability depending on the magnetic structure indicating magnon-phonon interactions. We are trying to find out how different magnetic structures affect the lattice vibration.

1. Elisabeth Sjöstedt, Lars Nordström, *Phys. Rev. B* 66, 014447 (2002)