Elastic stability of magnetic crystals under compression

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Stability of materials with magnetic ordering under various loading conditions and the influence of loading on the magnetism has been studied in many previous works. Some papers reported crystal phase transitions and a decay of magnetism during loading. Our work is aimed to study mechanical and magnetic stability of such materials under isotropic compressive and also tensile loading using proper analysis based on elastic moduli of the crystal system.

Elastic stability can be assessed via calculations of the total energy of the crystal system. The energy can be expressed as a function of deformation tensor in terms of elastic coefficients of first and second order. Elastic stability with respect to a deformation can be tested using small distortions from any reference state and corresponding change of crystal energy. In case of symmetric systems, the number of such independent deformations is limited and the stability analysis is possible.

The total energy will be computed by means of the Vienna ab initio simulation package (VASP). This code uses projector augmented-wave potential and plane wave basis set. The exchange and correlation contribution to the total energy will be treated by means of generalized gradient approximation. Magnetic ordering will be taken into account via spin polarized calculations.

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