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Elastic stability of magnetic crystals under isotropic compression and tension

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Abstract

Mechanical stability of Fe, Ni and Cr in their ground-state cubic structures has been tested under isotropic compressive and tensile loading using an analysis based on elastic moduli of the crystal system. This analysis has also been used to compute the theoretical strengths of the studied elements. Elasticity has been studied using small distortions from several reference cubic states and corresponding changes of crystal energy. The total energy has been computed by means of ab initio code that uses plane wave basis set. The exchange and correlation contribution to the total energy has been treated by means of generalized gradient approximation. Magnetic ordering has been taken into account via collinear spin polarization. No shear instability has been found in the region of tensile stresses up to the points of inflection on energy–volume dependencies of studied systems.

Keywords: Magnetism; Elastic moduli; Stability analysis; Isotropic loading

1. Introduction

Stability of materials with magnetic ordering under various loading conditions and the influence of loading on the magnetism have been extensively studied especially during the last decade [1–9]. First-principles calculations reported decay of magnetism under applied compressive loading [1,2,4,5,8,9]. It was also proved that magnetism can stabilize some crystal structures [2,7]. Some authors studied also mechanical instabilities and crystal phase transitions induced by changes of the magnetic moment [7]. It was shown that magnetism can also play a significant role in some pressure-induced phase transitions. One of the phase transitions of interest was the martensitic bcc–hcp transition in iron [1,3,9].

Our work is aimed to study mechanical and magnetic stability of Fe, Ni and Cr under isotropic compressive and tensile loading using an analysis based on elastic moduli of the crystal system. All the studied crystals are in their natural ground-state structures with corresponding ordering of spins; i.e. iron posses the bcc structure with ferromagnetic (FM) ordering, fcc nickel has also FM ordering and bcc chromium is considered to be of the anti-ferromagnetic (AFM) ordering of spins. This allows us to follow the whole deformation path to the point of instability and to evaluate the theoretical strength of each investigated crystal.

2. Computational details

2.1. Elasticity and stability

The elastic stability with respect to a deformation can be tested by applying small distortions from any reference state and computing the corresponding change of the crystal energy. In case of symmetrical systems, the number of such independent deformations is limited and the stability analysis is possible.

The crystal energy can be expanded in Taylor series (up to second-order term):

$$E_c = E_0 + V_c \sum_i \sigma_i \eta_i + \frac{1}{2} V_c \sum_i \sum_j C_{ij} \eta_i \eta_j + O(\eta^3) \qquad (1)$$

where V_c is the crystal volume, σ_i and η_i are components of the stress and strain tensors in the Voigt notation and C_{ij} are elastic moduli [10].

The elastic stability can be assessed in terms of the elastic moduli using an appropriate set of conditions [10,11]. In case of

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a cubic system, there are only three stability conditions:

$$C_{11} + 2C_{12} - \sigma > 0 \quad (2)$$

$$C_{11} - C_{12} + 2\sigma > 0 \quad (3)$$

$$C_{44} + \sigma > 0 \quad (4)$$

In order to test the stability conditions, one can perform a small distortion of crystal (a deviation from the main isotropic deformation path) and compute the corresponding combination of elastic moduli using the change of total energy [12].

The stability condition (2) corresponds to the requirement that the crystal is stable with respect to the volume expansion. It is related to the inflexion point on the dependence of total energy of the crystal on its volume and was tested in all above-mentioned previous calculations. The violation of stability condition (3) corresponds to a shear instability (vanishing of the tetragonal shear modulus) when we can expect the bifurcation from the primary deformation (isotropic) path to a secondary one (where the lattice acquires tetragonal or orthorhombic symmetry). The condition (4) corresponds to another shear instability related to the trigonal shear modulus. However, the above described stability analysis can check the crystal stability only with respect to homogeneous deformations.

In case of isotropic loading, the stress can be easily computed according to relation:

$$\sigma = \frac{\mathrm{d}E}{\mathrm{d}V} = \frac{1}{V}\frac{\mathrm{d}E}{\mathrm{d}v}$$

where E is the energy per atom, V the atomic volume and v is the relative volume.

2.2. Computational code

For the electronic structure calculations, we utilized the Vienna Ab initio Simulation Package (VASP) [13]. This code uses projector augmented-wave potential [14] and plane wave basis set. Cutoff energies for the basis set were 350, 350 and 295 eV for Fe, Ni and Cr, respectively. The exchange–correlation energy was evaluated using the generalized gradient approximation of Perdew and Wang [15] with Vosko et al. interpolation [16]. The $20 \times 20 \times 20$ k-points mesh was used in all our calculations. The solution was considered to be self-consistent when the energy difference of two consequent iterations was smaller than 0.1 meV. Magnetic ordering was taken into account via collinear spin polarization.

3. Computed results and discussion

Table 1 contains computed values of the equilibrium lattice parameter a_0, (1 Å $= 10^{-10}$ m) the bulk modulus B, the tetragonal $C' = (C_{11} - C_{12})/2$ and the trigonal C_{44} shear moduli and the magnetic moment μ along with experimental data [17,18]. The magnetic moment is expressed in Bohr magnetons μ_B.

As can be seen, the computed values of a_0 are mostly lower than those obtained experimentally, whereas the B values are slightly overestimated. A more significant discrepancy (up to 30%) can be found for values of tetragonal shear modulus. On the contrary, C_{44} values are underestimated. Computed values of magnetic moments μ agree mostly well with the experimental data. Only in case of Cr, the magnetic moment overestimates the experimental value of $0.62\mu_B$ [5]. On the other hand, the here reported value is lower than, e.g. the result ($1.1\mu_B$) of calculations of Guo and Wang [5].

Table 1
Computed values of the equilibrium lattice parameter a_0, the bulk modulus B, the tetragonal C' and trigonal C_{44} shear moduli (extrapolated to 0 K temperature) and magnetic moment μ

Quantity	a_0 (Å)	B (GPa)	C' (GPa)	C_{44} (GPa)	μ (μ_B)
Fe					
Calculated	2.83	190	67	99	2.20
Experimental	2.87	173	53	122	2.22
Ni					
Calculated	3.52	193	58	127	0.62
Experimental	3.52	188	55	132	0.60
Cr					
Calculated	2.85	199	188	86	0.90
Experimental	2.88	190	153	104	–

Fig. 1 displays magnetic moments μ as functions of atomic volume for Fe, Cr and Ni in their bcc and fcc ground-state structures with (anti-)ferromagnetic ordering of spins. In case of Cr, the internal magnetic moment per atom is displayed. The vertical lines correspond to volumes in equilibrium V_0 and at inflection point V_{ip} of the $E(V)$ function. The magnetic moments in all three cases decrease under compression and vanish at low volumes. The dependencies are consistent with those computed previously by means of LMTO-ASA [8]. Chromium exhibits a very strong volume-dependence of μ in the vicinity of the equilibrium volume. The magnetic moment of iron exhibits the steepest descent at the volume of about 6.7 Å^3.

In order to investigate the crystal stability and to be able to evaluate the theoretical strength, we plot left-hand sides of Eqs. (2)–(4) as functions of lattice parameter in the whole range of investigated volumes. Fig. 2 displays results of the stability analysis for iron, nickel and chromium crystals under hydrostatic loading in both tensile and compressive region of stress. In order

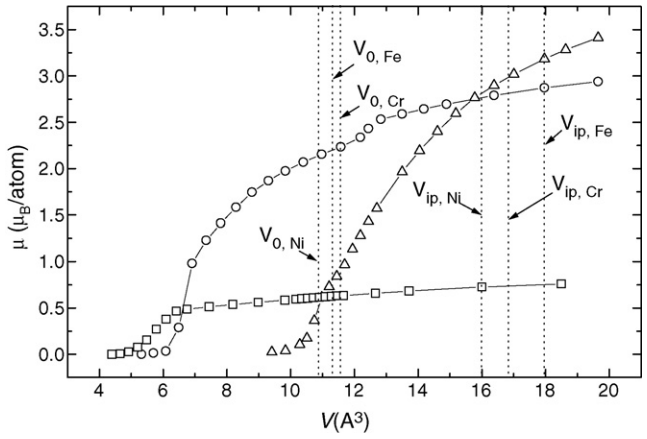

Fig. 1. Magnetic moments μ of Fe (○), Ni (□) and Cr (△) as functions of their atomic volume.