AB INITIO SIMULATION OF THREE-AXIAL DEFORMATION OF PERFECT IRON CRYSTAL

M. ČERNÝ[1,2], P. ŠANDERA[1] J. POKLUDA[1], M. FRIÁK[2,3] AND M. ŠOB[2]

[1]*Institute of Engineering Physics, Faculty of Mechanical Engineering*
Brno University of Technology, Technická 2, 616 69 Brno, Czech Republic
[2]*Institute of Physics of Materials, Academy of Sciences of the Czech Republic*
ikova 22, CZ616 62 Brno, Czech Republic
[3]*Institute of Condensed Matter Physics, Faculty of Science, Masaryk University*
Kotlářská 2, CZ-611 37 Brno, Czech Republic

ABSTRACT

Ab initio electronic structure calculations of ideal strength, bulk modulus and equilibrium lattice parameter of iron in the body-centered-cubic lattice under three-axial tension are performed using the linear muffin-tin orbitals method in atomic sphere approximation (LMTO-ASA) and the full-potential linearized augmented plane waves method (FLAPW). Magnetic ordering was taken into account by means of spin-polarized calculation. Two exchange-correlation energy approximations were employed, namely the local (spin) density approximation (LDA) and the generalized gradient approximation (GGA). Computed values are compared with experimental data.

KEYWORDS

Ab initio calculations, ideal strength, LMTO-ASA, FLAPW, spin polarization.

INTRODUCTION

Calculations of properties of materials exhibiting special magnetic properties as ferromagnetism or antiferromagnetism usually yield values different from experimental data when the magnetic ordering is omitted. The spin-polarization represents a possible way of including magnetism into ab initio calculations. The purpose of this paper is to compute ideal strength σ_{id} under three-axial tension using different ab initio approaches with and without spin polarization. As there are no experimental σ_{id} data available the reliability of individual ab initio approaches can be assessed by comparison of other predicted mechanical and structural characteristics with experimental values. Values of bulk modulus K, equilibrium lattice parameter a_0 and magnetic moment μ are very suitable for this purpose.

METHODOLOGY

All properties of interest were calculated from the dependence of the total energy E_{tot} on the relative volume ν. The Linear Muffin-tin Orbitals (LMTO) method in the framework of an Atomic Sphere Approximation (ASA) [1] and the Full-potential Linearized Augmented Plane Waves (FLAPW) [2] was applied for the total energy evaluation. The exchange-correlation contribution was evaluated within the local (spin) density approximation (L(S)DA) [3] and Generalized Gradient Approximation (GGA) [4].

The main approximations in the LMTO-ASA method are following: Potential and the total energies are calculated from spherically averaged charge densities and the Wigner-Seitz cell is approximated by a sphere. The basis consists of LMTO's of *s*-, *p*-, *d*- and *f*-symmetry. A mesh of 752 irreducible k-points is used. Other details of the calculations can be found in [5].

Within FLAPW no approximation (e.g. spheridization as in ASA) is used for description of both crystal potential and charge density. The electron wave functions are inside non-overlapping muffin-tin spheres expressed as a linear combination of radial functions (solutions of radial Schrödinger equation) multiplied by spherical harmonics and in the remaining space (interstitial region) are described by a linear combination of plane waves. The condition that basis functions inside the MT spheres must match the corresponding basis functions (plane waves) in the interstitial region on the sphere boundary in value and slope determines certain coefficients in the expression for the basis functions and such basis functions are called "augmented plane waves". The details of FLAPW calculations are described elsewhere [6].

RESULTS AND DISCUSSION

The $E_{tot}(a)$ functions obtained using both the spin-polarized calculations with ferromagnetic ordering (FM) and non-spin-polarized (nonmagnetic - NM) calculations are shown in Fig. 1. The curves in Fig. 1 were obtained by means of LMTO GGA. The LDA curves look qualitatively similar. The energy difference between the minima is 472 meV when using GGA and 227 meV when using LDA. Value of 286 meV obtained by KKR method [7] is in a better agreement with our LDA result since the approximation of the exchange-correlation term is the same as in [7]. One can also see that both curves overlap in the compression region. As expected, the critical merging point is associated with the vanishing of the magnetic moment μ (see Fig. 2). The corresponding pressure is about 170 GPa. As it was shown by Söderlind et al [8], however, the bcc $\rightarrow$ hcp phase transition is predicted at a pressure about 10 GPa, i.e. well before reaching the critical merging point discussed above. This result is also supported by experiment [9] where the observed pressure is somewhat higher.

Calculated values of equilibrium lattice parameter a_0, the ideal strength σ_{id}, the normalized lattice parameter related to the point of instability a_{ip}/a_0 and bulk modulus

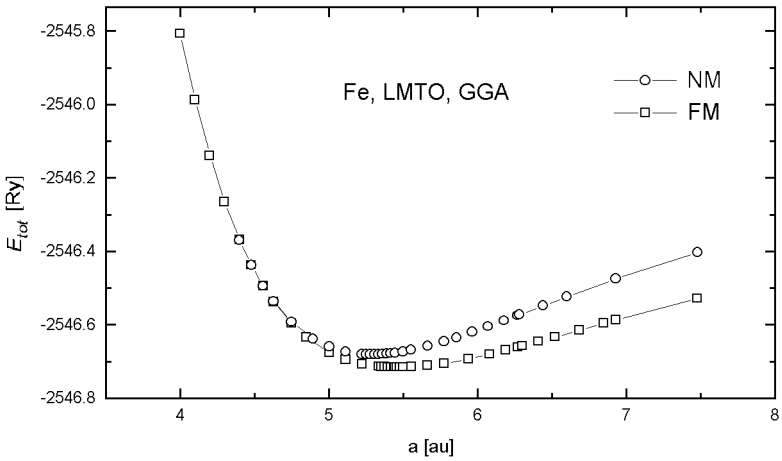

Figure 1: Total energy of iron atom as a function of lattice parameter

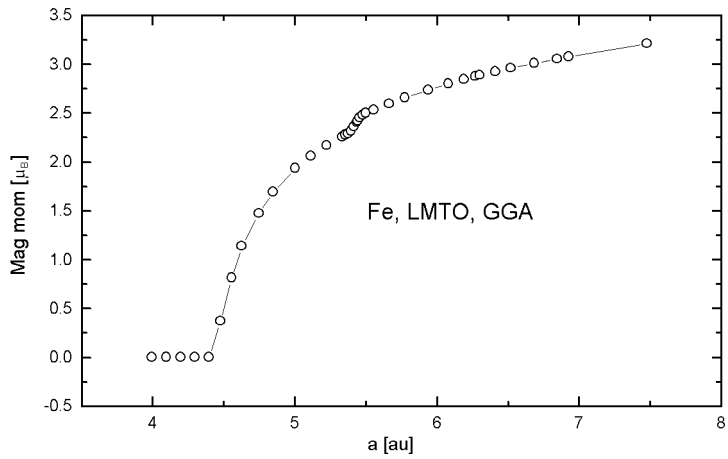

Figure 2: Magnetic moment of iron as a function of the lattice parameter

K are displayed in Tab. 1 and compared with experimental data [10, 11]. The value $K = 306$ GPa for non spin-polarized calculation published in [7] lies in between our LMTO LDA NM and LMTO GGA NM results. The reported value of 217 GPa for spin-polarized calculation and related values of equilibrium lattice parameter $a_0 = 2.79$ Å and magnetic moment $\mu = 2.15\,\mu_B$/atom are in a good agreement with experiment.

As can be seen from Tab. 1, our LMTO results exhibit similar trends. The magnetic moment obtained from the LMTO LDA calculations is lower than the experimental one and well comparable with FLAPW LDA result. On the other hand, LMTO GGA yields higher μ value unlike the FLAPW GGA exactly matching experiment. It should be noted, however, that LMTO GGA value becomes a slightly bit lower when computed at the experimental lattice parameter. Our value of $2.34\,\mu_B$ at experimental lattice constant is very close to $\mu = 2.32\,\mu_B$ obtained by Bagno et al [12] by means of LMTO-ASA method using GGA according to [13].

As expected, the FLAPW method yields results better than the LMTO-ASA one when compared with experiment. As this approach reprodeces the experimental value of μ (see

Table 1: Computed characteristics of iron

property	LMTO-ASA				FLAPW FM		experiment
	LDA NM	GGA NM	LSDA FM	GGA FM	LDA	GGA	
a_0 [Å]	2.70	2.79	2.75	2.88	2.78	2.85	2.87
a_{ip}/a_0	1.14	1.15	1.16	1.16	1.16	1.16	-
K [GPa]	339	260	257	128	229	186	173
σ_{id} [GPa]	52.8	39.8	37.8	26.6	28.5	34.9	-
μ [μ_B]			2.04	2.42	2.04	2.22	2.22

Tab. 1), it may be concluded that the non-spherical effect must be properly included when we wish to describe the magnetic behavior correctly.

ACKNOWLEDGEMENTS

This research was supported by the Ministry of Education of the Czech Republic (Research Plan No. MSM262100002), the Grant Agency of the Academy of Sciences of the Czech Republic (Project No. A1010817), and by the Grant Agency of the Czech Republic (Project No. 106/99/1178). The use of the computer facility at the MetaCenter of the Masaryk University, Brno is acknowledged.

REFERENCES

[1] Krier G., Jepsen O., Burkhardt A. and Andersen O.K.: The TB-LMTO-ASA Program, version 4.6. Max-Planck-Institut für Festkörperforschung, Stuttgart, 1994.

[2] P. Blaha *et al.*, WIEN97, Technical University of Vienna 1997 (improved and updated Unix version of the original copyrighted WIEN-code, which was published by P. Blaha *et al.*, in Comput. Phys. Commun., 59, 399 (1990)).

[3] Barth V., Hedin L.: J. Phys. C : Solid State Phys. 5 (1972), 1629.

[4] Perdew J. P., Wang Y.: Phys. Rev. B 45 (1992), 13244.

[5] Černý M., Šandera P., Pokluda J.: this proceedings.

[6] Friák M., Šob M., Vitek M.: this proceedings.

[7] Moruzzi V. L., Janak J. F., Williams A. R.: Calculated Electronic Properties of Metals, Pergamon Press, New York 1978.

[8] Söderlind P., Moriarty J. A., Wills J. M.: Phys. Rev. B 53 (1996), 14063.

[9] Wang F.M., Ingalls R.: Phys. Rev. B 57 (1998), 5647.

[10] Kittel C.: Introduction to Solid State Physics, John Wiley & Sons, New York, 1976.

[11] Landolt-Börnstein: Numerical Data and Function Relationships in Science and Technology. NS, Gr. III, Vol. 2 Eds. K.H. Hellwege and A.M. Hellwege, Berlin - Heidelberg - New York, Springer, 1971.

[12] Bagno P., Jepsen O., Gunnarson O.: Phys. Rev. B 40 (1989), 1997.

[13] Perdew J. P., Wang Y.: Phys. Rev. B 33 (1986), 8800.