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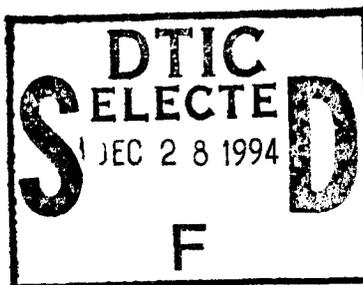


A New Method of Evaluating The Explicit Magnetic-State-Dependent Energy In Semi-Emperical Calculations on Iron

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13. ABSTRACT (Maximum 200 words) The existing semi-empirical methods for use in atomic computer simulations in iron (such as various modifications of the Embedded Atom Method) have not explicitly taken account of the ferromagnetism <i>per se</i> . Rather, the adjustable parameters just have been fitted to mechanical and thermal properties of iron. However, when the magnetic properties are essential in affecting localized atomic behavior (e.g. in the vicinity of crystal defects), these methods may be inadequate. To remedy the situation, a procedure is suggested of explicitly calculating the magnetic contribution to the energy of individual atoms, as a function of their atomic environment. The method uses the Stoner approach, as previously developed in, and a data base obtained by the LMTO-Stoner calculations on BCC Fe under hydrostatic and tetragonal deformations, and Fe free surfaces. The procedure may be incorporated in any semi-empirical method: the ferromagnetic contributions to the bulk moduli, C_{11} , C_{12} and C_{44} are easily calculated and may be subsequently used in adjusting the semi-empirical method parameters. Preliminary testing shows a good agreement with the magnetic properties obtained by the LMTO-Stoner calculations.				
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Introduction

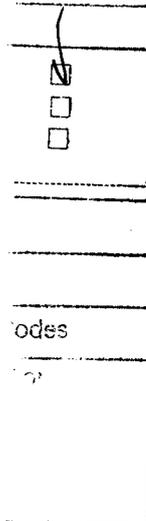
During the recent decade, iron has been the object of extensive study by various first principles methods (for references and comparison of results for iron obtained by different methods see, e.g. [1-4]). However, the self-consistent spin-polarized calculations on BCC iron inevitably failed to predict the relative stability of the ferromagnetic (FM) BCC phase with respect to the nonmagnetic (NM) FCC (see discussion in [4]). This failure is believed to be mainly due to the local spin-density approximation used in the calculations.

Because of this fundamental difficulty, at the present time, an entirely *ab initio* analysis of structural phase transformations in iron is impossible. However calculations, which do not require comparison of energetics of different phases, like modeling of grain boundaries and free surfaces, can be successfully performed [5-7]. An alternative approach to the totally *ab initio* analysis is to introduce into the theory an adjustable parameter in order to make calculations more consistent with experimental observations.

Along this path, in Refs. [8-10], we have chosen to calculate the equilibrium magnetic moments as well as the magnetic contributions to the ground state energies of iron using the Stoner model of itinerant ferromagnetism [11], rather than performing spin-polarized calculations. The Stoner exchange parameter, I , can then serve as an adjustable parameter. Having made only one adjustment, such a procedure enabled us to perform the complete analysis of the relative stability of BCC and FCC phases, as well as the energetics of the BCC-FCC lattice deformation in iron.

In spite of the tremendous success in development, in the recent decade, of new first-principles methods of modeling, as well as efficient computer codes and proliferation of powerful high-speed computers, a totally first-principles modeling of important processes fundamentally affecting the mechanical properties of metallic alloys, is too computationally intensive and therefore practically impossible.

In response to the pressing necessity of filling this void, the efficient semi-empirical methods, such as different versions of the so-called Embedded Atom Method (EAM)[12], or Angular Force Method (AFM)[13], have been developed.



However, the existing semi-empirical methods for use in atomic computer simulations in iron still have not explicitly taken account of the ferromagnetism *per se*. Rather, the adjustable parameters just have been fitted to mechanical and thermal properties of iron. At the same time, when the magnetic properties are essential in affecting the atomic behavior (e.g. in the vicinity of crystal defects), these methods may be inadequate.

To remedy the situation, we suggest the procedure of explicitly calculating the magnetic contribution to the energy of individual atoms, as a function of their atomic environment. This procedure is based on the Stoner theory of itinerant ferromagnetism, and uses the information that has been accumulated in our earlier research on iron, mentioned above.

The plan of this paper is as follows. In Sec. 2 we discuss the Stoner model of itinerant ferromagnetism. In Sec. 3, we discuss the parametrization of the the ingredient quantities to be used in semi-empirical calculations. Sec. 4 summarizes the procedure and discusses potential applications of the new method to EAM and AFM.

The Stoner Model of Itinerant Ferromagnetism

The Stoner theory, first suggested in 1939 [11], has been successfully used in recent years in estimating both the equilibrium magnetization and magnetic energy of band electrons. This was made possible as a result of a rigorous formulation of the Stoner model as a perturbation approach in terms of microscopic electronic theory [14-17]. Particularly, the fundamental parameter of the theory, the Stoner exchange parameter, I , was understood in terms of density-functional characteristics. In iron, the theory explained the metamagnetic behavior of the FCC phase [14,18,7]. The Stoner approach in combination with self-consistent non-spin-polarized calculations enables one to perform the detailed analysis of ferromagnetic (FM) behavior, as well as identify all the possible magnetic stationary phases: both stable, metastable and even unstable, and find the areas of their emergence. Such an analysis, using traditional spin-polarized calculations is at present either too cumbersome and practically impossible.

The Stoner model in its original formulation postulates that the change of energy upon forming a FM state with moment \mathbf{m} consists of two parts. The first is the exchange energy contribution, $-1/4 I \mathbf{m}^2$, where the exchange parameter I is a constant. The second, the kinetic energy term is found by forming two subbands for spin up and down electrons by flipping $\mathbf{m}/2$ spin down electrons

from just below the non-magnetic (NM) Fermi level into the unoccupied spin-up states just above the Fermi level. As was shown in [14-17], this procedure corresponds to the first order perturbation theory in \mathbf{m}/n_V (n_V is the number of valence electrons per atom). Thus, for a given \mathbf{m} , the magnetic contribution to the total energy is:

$$E_m = \frac{1}{2} \int_0^{\mathbf{m}} \mathbf{m}' / N(\mathbf{m}') d\mathbf{m}' - \frac{1}{4} I \mathbf{m}^2 \quad (1)$$

where $N(\mathbf{m})$ is the NM density of states averaged between the Fermi levels of spins up and down electrons as found from the rigid subband shift. The procedure of 'constructing' $N(\mathbf{m})$ is illustrated in Fig. 1.

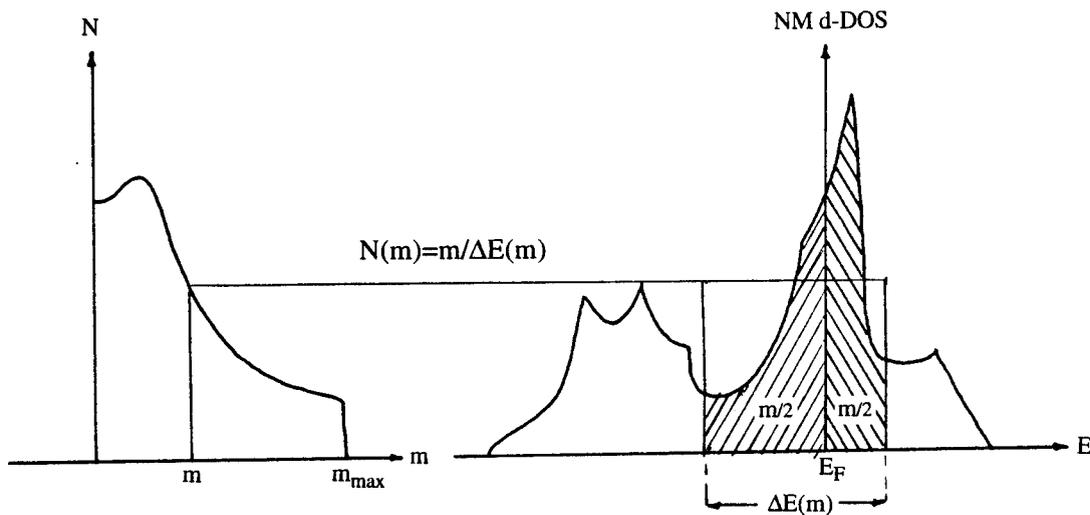


Fig. 1. Schematic construction of the $N(\mathbf{m})$ function.

The stationary state requirement :

$$\partial E_m / \partial \mathbf{m} = 0,$$

gives, apart from the "trivial" solution, $\mathbf{m}=0$, the criterion for arising a FM state:

$$I \cdot N(\mathbf{m}) = 1 \quad (2)$$

Suppose Eq. (2) has a solution, \mathbf{m} . Then the corresponding FM state is stable ($\partial^2 E_m / \partial \mathbf{m}^2 > 0$) if

$$\partial N(\mathbf{m}) / \partial \mathbf{m} < 0 \quad (3)$$

otherwise it is unstable ($\partial^2 E_m / \partial \mathbf{m}^2 < 0$). However, even if Eqs. (2,3) hold, the FM state may not occur if $E_m > 0$. In this case the FM state is metastable.

As for the NM state, $\mathbf{m}=0$, it is stable and may coexist with a FM state (metamagnetic situation), only so far as

$$[\partial^2 E_m / \partial \mathbf{m}^2]_{\mathbf{m}=0} > 0 \quad (4)$$

or, equivalently,

$$I N(E_F) < 1 \quad (5)$$

where $N(E_F)$ is the NM density of states (DOS) at the Fermi level ($N(E_F)=N(0)$).

From the perturbation theory analysis [14-17], I can be found in terms of the NM system. From the linear response theory [17] it follows:

$$I = \int d^3r \gamma^2(r) |K(r)| \quad (6)$$

(the three-dimensional integral is taken over the whole volume of crystal) where

$$\gamma(r) = \frac{\sum_{i,j} \delta(E_F - E_i) |\psi_i(r)|^2}{N(E_F)}$$

and

$$K(r) = 1/2 [d^2 E_{xc}(r, \mathbf{m}) / d\mathbf{m}^2]_{\mathbf{m}=0}$$

Here E_i , $\psi_i(r)$ are respectively the eigenvalues and the wave functions of the NM system; $E_{xc}(r, \mathbf{m})$ is the exchange-correlation functional.

An important property of the averaged DOS $N(\mathbf{m})$ is that, being multiplied by the d-electron "band width", W , it happens to be virtually independent of volume, or the Wigner-Seitz (WS) radius, s . Then Eq. (2) reads:

$$N(\mathbf{m}) = W(s)/I(s) \quad (7)$$

Where $N(\mathbf{m}) = W * N(\mathbf{m})$. Fig. 2 shows $N(\mathbf{m})$ curves for two s values. The right-hand side of the above Eq. does depend on s , and this dependence is important.

Until recently, the Stoner parameter, I , has been believed to be essentially a constant, independent of both the volume and the crystal structure of the metal. Our calculations on both the BCC and FCC iron [8-10] revealed the monotonic,

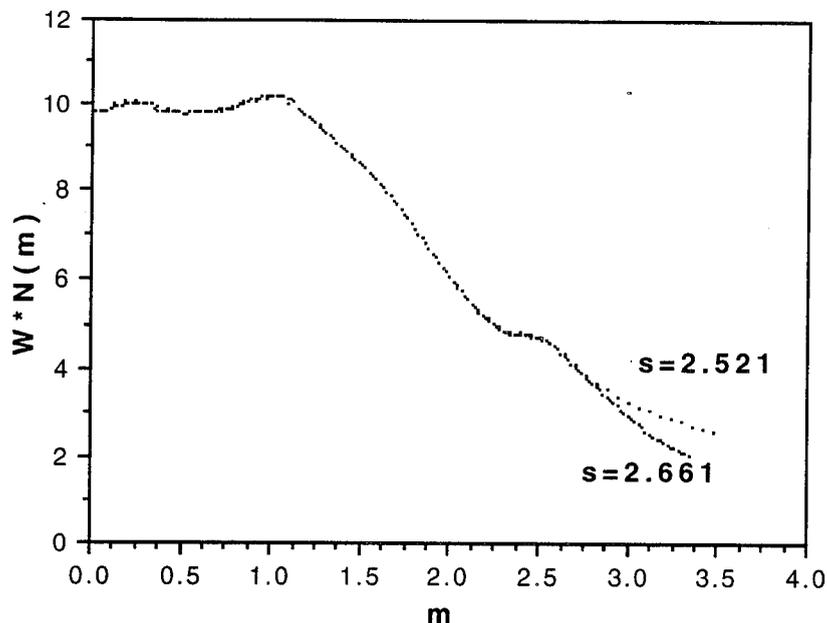


Fig. 2. $N(\mathbf{m})$ s for BCC lattice for two WS radii.

though rather weak, dependence of I on the WS radius, s . Both the magnetic energy, Eq.(1), the equilibrium magnetic moment, \mathbf{m} , (as found from Eq. (2)), and the equilibrium atomic volume, happen to be rather sensitive to the values of I . The idea of papers [8-10] was to adjust the value of I , so that the equilibrium WS radius, s_0 , for the FM BCC phase be equal to the experimental value. In Table I we compare the calculated s_0 , for $I = \beta I_0$ [where I_0 is the "ab initio" value, Eq. (6), and $\beta=1.000, 1.025, 1.050, 1.075$ and 1.090]. One can see that for $\beta=1.075$, the equilibrium WS radius, $s_0=2.659$ a.u., almost matches the experimental value. Therefore, we have chosen $\beta=1.075$ as the "universal" enhancement factor; all the calculations in [9] for the whole range of c/a values were done with this β . No other adjustments of any parameters were performed.

Table 1.
Dependence of the equilibrium WS radius for the FM BCC phase on the Stoner parameter enhancement factor, β .

β	1.000	1.025	1.050	1.075	1.090
s , a.u. ^a	2.648	2.650	2.654	2.659	2.664

a) Experimental value, $s=2.661$ a.u. (Ref. [19])

We used the LMTO method [20] with the so-called combined correction term [20], and the Madelung electrostatic correction [21]. Scalar relativistic calculations on uniform meshes of 1540 points in the irreducible wedges of BCT Brillouin zones were done, with the exchange-correlation functional of von Barth and Hedin [22]. Also, the frozen core approximation was used [23].

Our calculations were done for 12 c/a -values : $1.0 \leq c/a \leq \sqrt{2}$. For each c/a , self-consistent non-spin-polarized calculations were performed for 9 values

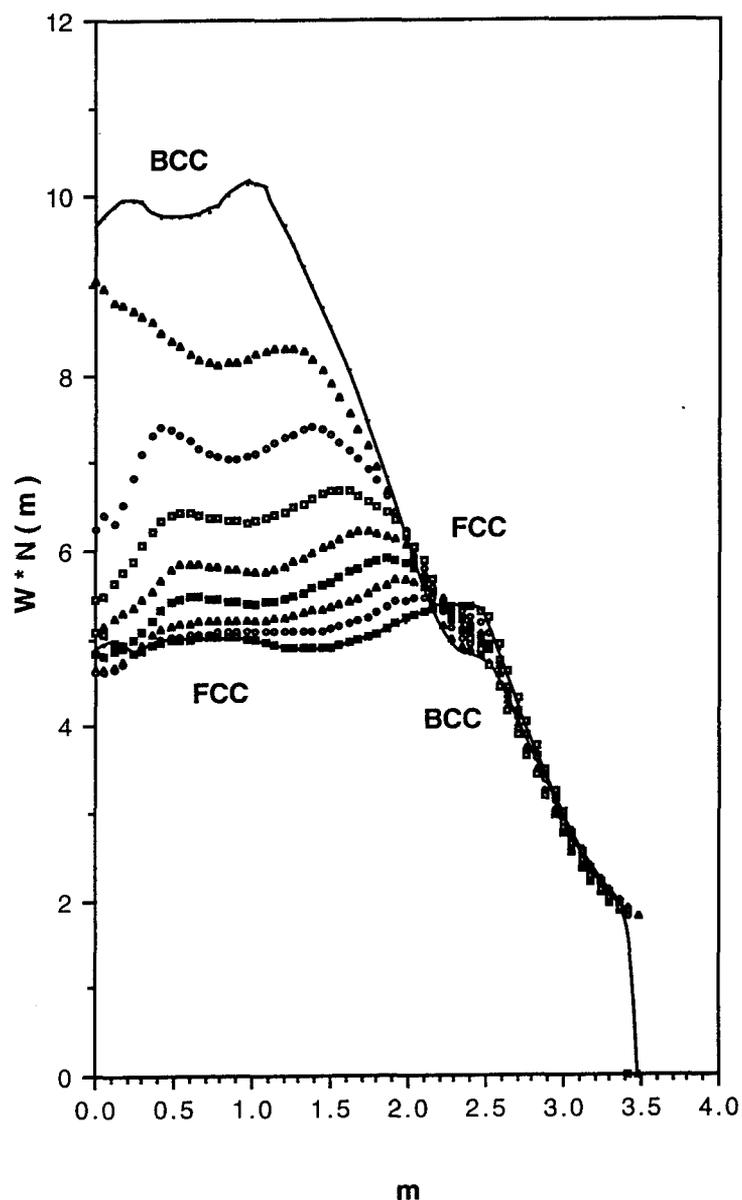


Fig. 3. The $N(\mathbf{m})$ functions for FCT lattices. Solid lines are the BCC and FCC curves. The other curves correspond to the intermediate c/a values.

of the WS radius, s ($2.521 \text{ a.u.} \leq s \leq 2.788 \text{ a.u.}$). In each calculation, after convergence had been achieved, the Stoner parameters, $I_0(c/a, s)$, Eq.(6), and then $I = 1.075I_0$ were found and the averaged DOS, $N(\mathbf{m})$ was generated. Then the Stoner equation, Eq.(2), was solved for the equilibrium magnetic moment, \mathbf{m} , and the magnetic energy E_m . The data base generated in this series of calculations will be used in our new method. Fig. 3 shows the $N(\mathbf{m})$ curves for BCT lattice.

The above data, however, reflect only the tetragonal deformation. An important ingredient of the new method, which is to be used in modeling GBs and free surfaces, should be information on free surfaces. The necessary data were provided by Dr. R. Wu of Northwestern University, whose work in Prof. Art Freeman's group, has been a part of the SRG effort.

In the next section we

will describe in detail the parametrization of the data and discuss the algorithm of the method.

Parametrization of the First-Principles Data and the Method Algorithm.

Using the Stoner model with the adjusted exchange parameter, we have calculated the structural properties of BCC and FCC iron and, for the first time, the energetics of the intermediate states along the Bain deformation path .

Any semi-empirical method has to be able to somehow describe the environment of the atom of interest. It is known from a vast experience of tight-binding calculations (see, e.g.[24]), that the number of neighbors is an important parameter which plays a crucial role in band-structure calculations. We have chosen, therefore, to introduce the so-called "effective number of neighbors", Z_{eff} , to allow for the atomic environment. Since all the quantities are to be parametrized in terms of Z_{eff} , its definition is not very critical. It is important, however, that Z_{eff} should reflect the real atomic environment. We define

$$Z_{\text{eff}} = \sum (R_{\text{min}}/R)^5 \exp(1-(R/R_{\text{min}})^2) \quad (8)$$

where the summation is over atom coordinates R (R_{min} is the distance from a given atom to its nearest neighbor). No cut-off radius is introduced, but, in fact, the exponential provides a rather fast sum convergence. Fig. 4 shows the dependence of Z_{eff} on c/a in body-centered tetragonal (BCT) lattices. One can see, that Z_{eff} for BCC and FCC equal respectively to 10.37 and 12.63, while the corresponding nearest neighbor numbers are 8 and 12. The 10.37 number actually reflects the fact that the 6 second nearest neighbors in the BCC lattice are also situated rather close to the first nearest neighbors ($R_{2\text{nd}}/R_{1\text{st}}=1.155$); in the FCC lattice they are farther away ($R_{2\text{nd}}/R_{1\text{st}}=1.414$). Therefore the 6 second nearest neighbors in the FCC lattice are less important giving a smaller contribution to Z_{eff} .

Apart from the "environment" or "structure" parameter, Z_{eff} , an important parameter is the volume per atom. In a perfect lattice the atomic volume, or, equivalently, the WS sphere of radius, s , can be easily found. In a deformed crystal, or a crystal with defects, the atomic volume is difficult to define, and, in fact it is a "bad" parameter.

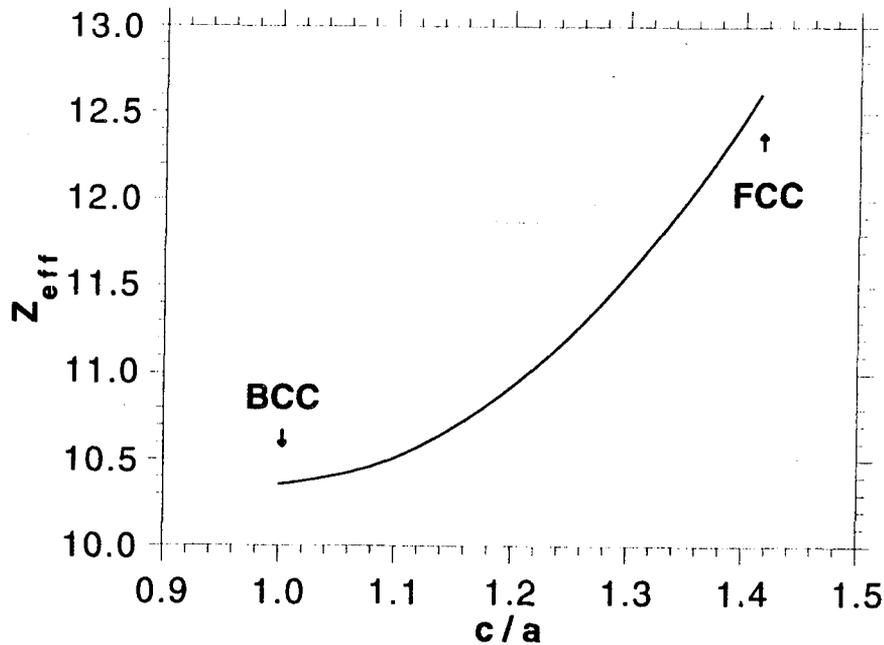


Fig. 4. Z_{eff} (c/a) for BCT lattice.

As was mentioned above, the left-hand side of Eq. (7), $N(\mathbf{m})$, virtually does not depend on s . However, the right-hand side does depend on s , where this dependence is mostly due to the d -electron band width, W .

It is known (see, e.g., [24]), that in perfect crystals $W \sim 1/s^5$. Therefore, it is convenient to parametrize W in the form:

$$W = A(Z_{\text{eff}}) (\sum 1/R^{10})^{1/2} \quad (9)$$

As a result, W has the right volume dependence.

The values of W are found as a by-product of first-principles calculations: our data base contains the values for a number of BCT lattices, as well as the BCC (111) free surface. Fig. 5 shows the results of fitting the function, Eq.(2) to the calculated W 's. The function $A(Z_{\text{eff}})$ is approximated by a polynomial in the interval $5.2 \leq Z_{\text{eff}} \leq 12.61$ (note the Z_{eff} values between 5.2 and 10.354 correspond to the (111) free surface).

We assume that the Stoner parameter, I , is only weakly volume dependent. However, it does depend on atomic environment, i.e. on Z_{eff} . We approximated the values of I , Eq. (6) (as found from the first-principles calculations, and augmented by factor 1.075; see section 2) by two polynomials in Z_{eff} (Fig.6).

Thus, if $N(\mathbf{m})$ is known, then, for a given Z_{eff} and W , the equation Eq. (7) can be solved for the magnetic moment, $\mathbf{m}=\mathbf{m}(W/I)$. The next step is calculating E_{kin} , the kinetic energy contribution (the integral in Eq. (1)), and then the total ferromagnetic energy, E_{m} .

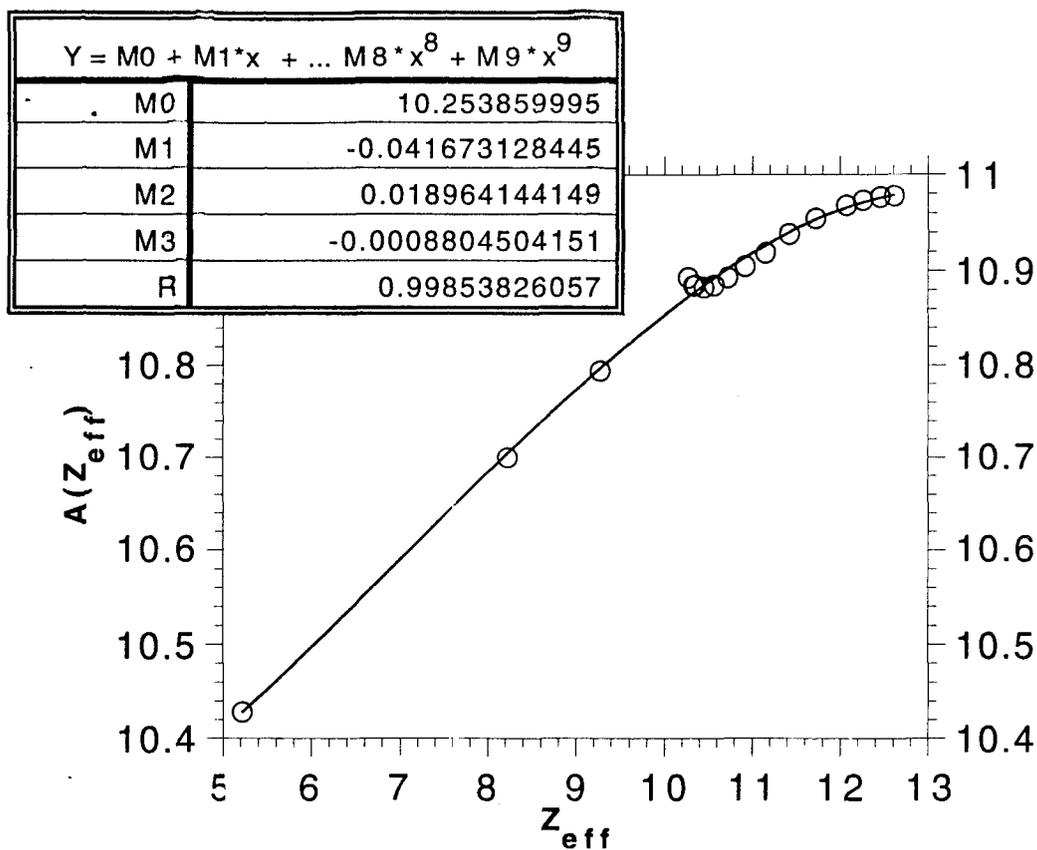


Fig. 5. Factor $A(Z_{eff})$ as a polynomial of Z_{eff} .

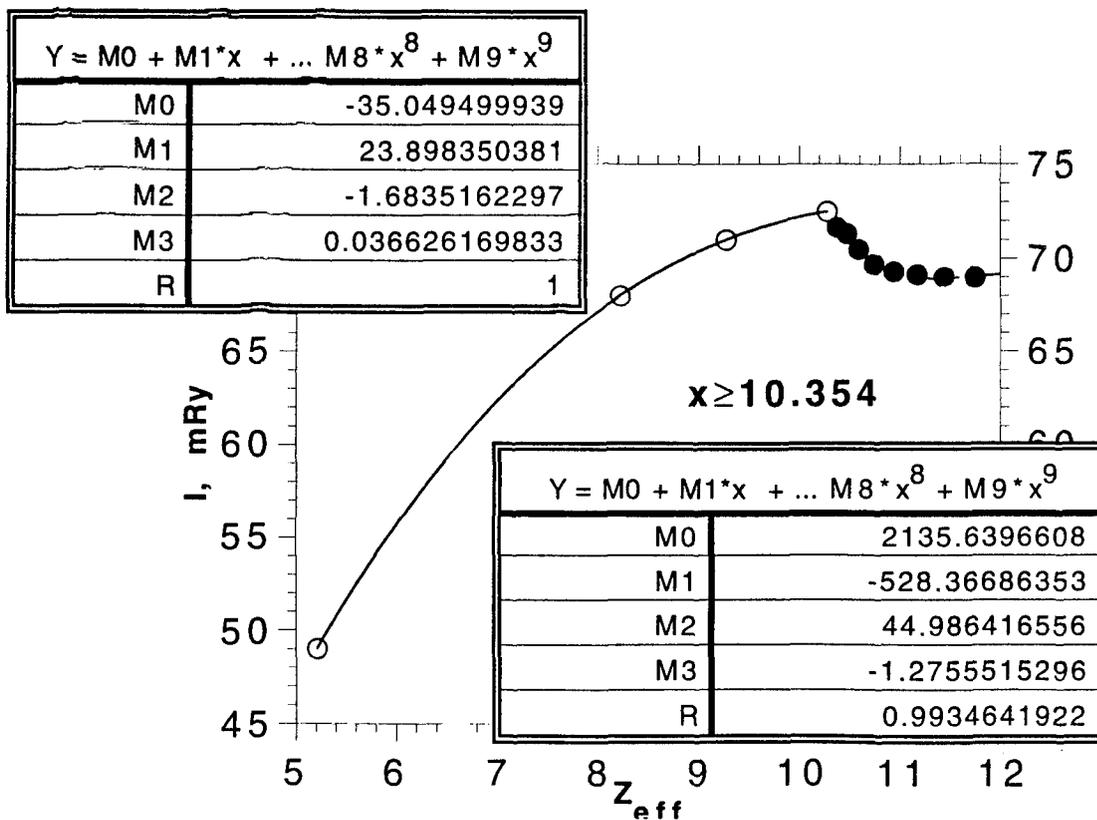


Fig. 6. The Stoner parameter, I , as approximated by two polynomials in Z_{eff}

Both the $N(\mathbf{m})$, $\mathbf{m}(x)$, $x=W/I$, and $E_{\text{kin}}(\mathbf{m})$ can be directly introduced into the computer code as DATA statements. The three data sets are the two-dimensional arrays, Z_{eff} being the second variable. It is known, that ferromagnetism is unstable beyond a definite range of atomic volume/structure values. This translates into a definite restriction for the values of $x=W/I$. The maximal allowable value of x as a function of Z_{eff} is shown in Fig.7.

Following the above prescription, the computer code was developed, in the form of subroutine STONER(ni, ri, amag, emag).

The procedure of calculations is as follows. The subroutine STONER is called from a main program which generates ni and ri, the total number of neighboring atoms and their distances from the atom of interest (ni should include as many atoms as it may be necessary for the Z_{eff} to converge), and amag and emag are the output magnetic moment on the atom of interest and its ferromagnetic energy.

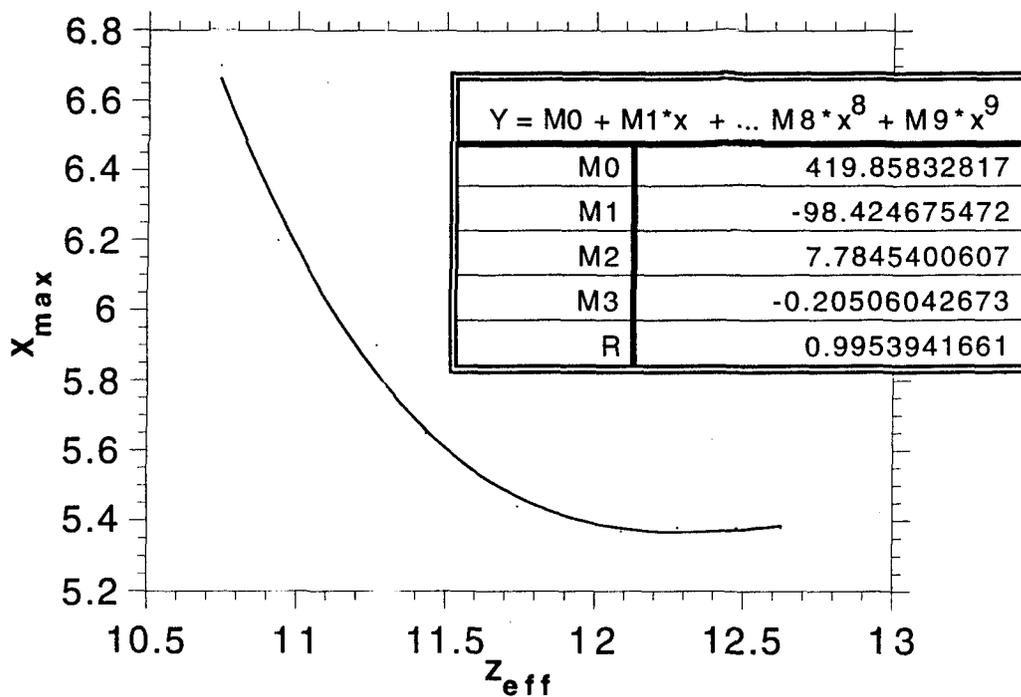


Fig. 7. The maximal value of parameter $x=W/I$, at which the ferromagnetic solution becomes unstable, as a function of Z_{eff} .

In the subroutine, first the Z_{eff} and W (using function $\text{fac}(z)$ which stands for $A(Z_{\text{eff}})$) are calculated, then the Stoner parameter $I(Z_{\text{eff}})$ and W/I are found for a given Z_{eff} . The next step is solving Eq. (7) for the magnetic moment \mathbf{m} -- simply reading the value from the corresponding array using two-dimensional interpolation. After finding \mathbf{m} , the kinetic energy, $E_{\text{kin}}(\mathbf{m}, Z_{\text{eff}})$, is found again

by two-dimensional interpolation (the interpolation subroutine is included in the code). Fig. 8 shows the E_{kin}/W plots for BCC, $c/a=1.24$ and FCC. The last step is calculation of the ferromagnetic energy:

$$E_m = E_{\text{kin}} - 1/4 I m^2 \quad (10)$$

Wherever Eq. (7) does not have a ferromagnetic solution (the ferromagnetic solution is unstable), or E_m is positive (the ferromagnetic solution is metastable), the subroutine returns the values $m=0.$, and $E_m = 0$.

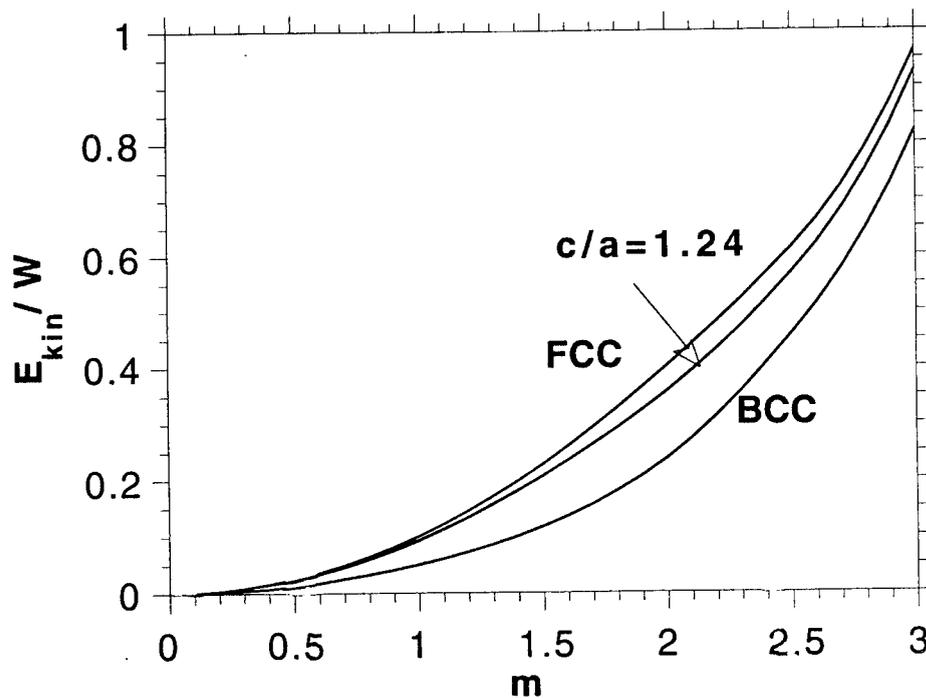


Fig. 8. The E_{kin}/W plots for BCC, $c/a=1.24$ and FCC

The test runs of the subroutine for BCT lattices for $s=2.661$ (equilibrium volume for BCC Fe) from $c/a=1.0$ (BCC) through $c/a=1.32$ (at higher c/a at this volume the ferromagnetic state is unstable) showed an excellent agreement between the values of m and E_m calculated by the new method and the results of the LMTO calculations (the only exception is $c/a=1.32$, where the energy is already quite small). Table 2 compares these results.

Table 2
Comparison of values of m and E_m as calculated by the new procedure and by the
LMTO first-principles method

c/a	m^{calc} (μ_B)	m^{LMTO}	E_m^{calc}	E_m^{LMTO} (mRy)
1.00	2.235	2.223	-30.39	-30.14
1.08	2.251	2.253	-25.34	-25.46
1.12	2.273	2.266	-20.93	-20.84
1.16	2.299	2.291	-15.79	-15.53
1.20	2.274	2.264	-10.35	-10.19
1.24	2.309	2.335	-5.987	-6.103
1.28	2.370	2.365	-2.924	-2.938
1.32	2.446	2.433	-0.277	-0.095

Potential Applications of the New Method in AFM and EAM

The new procedure can be easily adopted by any semi-empirical method. The most popular method, the EAM, in its various modifications, fits some of the calculated quantities to their experimental values. In all EAM versions, among those quantities are the bulk modulus and the three elastic moduli: C_{11} , C_{12} and C_{44} .

In order to implement the new procedure, a series of calculations for hydrostatic, tetragonal and monoclinic (or triclinic) deformations of BCC Fe have to be performed, and the ferromagnetic contributions to the corresponding elastic moduli found. Then, this information is to be used in fitting the adjustable parameters in the corresponding EAM.

Originally, it was planned to implement the new procedure to the recently developed AFM. The validity and advantages of the AFM were then to be tested on the ferromagnetic Iron. However, the results of our recent calculations [25], using the AFM for modeling the relaxation of a grain boundary in tungsten, appear to be somewhat doubtful.

Our previous investigation using the so-called Finnis-Sinclair modification of the EAM [6] for GB relaxation in tungsten, discovered an anomalous relaxation of the third (from the GB plane) plane of W atoms, the so-called " ω -phase effect". It was also observed in Fe by the EAM simulation [26], our Finnis-

Sinclair calculations [27], and restricted relaxation calculations using the first-principles method [7]. However, this effect, which is easily understood from the physical point of view [6], was not obtained in the AFM GB relaxation in W. This negative result has suggested that the detailed analysis of the AFM should be put on hold. Instead, the emphasis should be given to the implementation of our new procedure to a more traditional version of EAM, recently developed by the author. This project will be carried out shortly.

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