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# The influence of boron impurities on the electronic states and magnetic behaviour of BCC iron: self-consistent LMTO recursion calculations

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**Abstract.** The generalization of the tight-binding linear-muffin-tin-orbital recursion method for impurity electronic-structure calculations, which takes into account the influence of the nearest-neighbour atoms in self-consistent way, is presented. The calculations for boron impurities in BCC iron have been performed and used for the investigation of magnetic behaviour of iron atoms in four nearest-neighbour shells. It is shown that the impurity significantly influences the states of first coordination shell atoms, but does not significantly change their magnetic moments. The mechanisms of magnetic interactions between the impurity and the matrix are discussed, based on the calculated results.

## 1. Introduction

As is known, iron usually contains the impurities of light s and p elements, such as boron, carbon, phosphorus and silicon, which can considerably influence its physical and chemical properties, including the magnetic ones. Because of this a large number of papers have been devoted recently to the electronic structure studies of different s and p impurities in BCC and FCC iron [1-3]. However, boron impurities in iron have not been considered in detail, though boron is known to be quite a common doping element in various transition metals and their alloys, and often leads to unusual and interesting properties, for example, 'boron ductility' observed in some alloys of transition metals [4], or the stabilization of amorphous transition metals and alloys with boron impurities.

Boron easily forms binary amorphous alloys with iron of the  $\text{Fe}_{100-x}\text{B}_x$  type in a wide range of concentrations,  $9 < x < 90$ , but its solubility in crystalline BCC iron is very low: 0.15% at 915 °C [5]. It has been established [5] that, unlike carbon, boron atoms in BCC iron occupy the substitutional positions. A number of ordered phases, such as FeB,  $\text{Fe}_2\text{B}$  and metastable  $\text{Fe}_3\text{B}$  are formed between boron and iron; each of these has different surroundings for boron atoms formed by the nearest iron neighbours. This in turn differs from the typical nearest-neighbour environment for a boron impurity in BCC iron. Such differences may result in differences in physical and chemical properties of these alloys, and especially their magnetic characteristics. The experimental data available [6, 7] show that boron usually decreases the value of magnetic moments of iron atoms. For example, in the  $\text{Fe}_2\text{B}$  alloy, where each boron atom is surrounded by eight nearest iron neighbours as in BCC iron, a saturation magnetization of  $1.9\mu_B$  has been obtained in the experiments [6]. However, such a decrease from the value  $2.2\mu_B$ , typical of pure iron, does not result in any other changes of its magnetic behaviour.

Great progress in the investigation of the electronic structure of impurities has been achieved due to the development of the Green function (GF) method based on the Korringa–Kohn–Rostoker (KKR) band-structure scheme [8, 9] or the linear-muffin-tin-orbital (LMTO) technique [10, 11]. At the early stage, calculations of impurity electronic structure were usually performed within the scope of the single-site approximation, where the perturbation of the crystal potential was taken into account in a self-consistent way for the impurity site only, and the host crystal was considered to be unperturbed. This is a very crude approximation which does not describe impurity energy parameters and their influence on the magnetic structure of the host crystal. These drawbacks have been overcome recently [12–15] within the scope of the KKR–GF approach, when the interactions of impurities with up to four or more nearest-neighbour shells were calculated self-consistently. Such calculations, being highly precise, are very difficult to implement for complicated impurity systems and require large amounts of computer time.

These difficulties are much less severe when the calculations are performed in real space without the requirement of translational symmetry. Such an approach has been developed recently in [16, 17] and is based on the combination of the recursion method and the LMTO method in the tight-binding representation (LMTO–TB–REC method). It allows self-consistent first-principles calculations in the local-spin-density approximation (LSDA) [21]. The detailed description of the LMTO–TB–REC method for the case of a non-magnetic topologically disordered system is given in [17]; its generalization for magnetic solids is presented in [16].

In the present paper we give a generalization of the LMTO–TB–REC method for impurity systems that allows us to take into account the impurity influence on the nearest-neighbour atoms in a self-consistent way. The method is used for the study of the electronic structure of a single boron impurity in BCC iron, and the influence of such an impurity on the electronic states of iron atoms in four nearest coordinational shells is investigated.

## 2. Method of calculations

In order to avoid the computational difficulties of band-structure approaches when applied to a system with broken translational symmetry, real-space methods can be used for the electronic-structure calculations. One of the most effective of these is the recursion method [18], which is based on the transformation of the one-electron Hamiltonian matrix to the tridiagonal form. Such a recursion procedure can be applied with the orthogonal and short-ranged Hamiltonian that can be built from first principles within the scope of the LSDA making use of the LMTO–TB representation [19, 20], and is as follows:

$$H_{iL,jL'}^{(1)} = C_{iL}^\alpha \delta_{ij} \delta_{LL'} + (\alpha_{iL}^\alpha)^{1/2} S_{iL,jL'}^\alpha (\alpha_{jL'}^\alpha)^{1/2} \quad (1)$$

where  $i$  and  $j$  denote the atomic positions, and  $L = (l, m)$  are the angular momentum indices.  $C^\alpha$  and  $\alpha^\alpha$  are the potential parameters,  $S^\alpha$  are the screened structure constants, representing the structure-dependent part of the Hamiltonian. The matrix elements  $S^\alpha$  can be calculated through the Dyson-type matrix equation

$$S_{iL,jL'}^\alpha = S_{iL,jL'}^0 + \sum_k \sum_{L''} S_{iL,kL''}^0 \alpha_{kL''}^\alpha S_{kL'',jL'}^\alpha \quad (2)$$

To first order in energy the Hamiltonian (1) is orthogonal. The potential part of the Hamiltonian can be determined using the LSDA.

The main problem of the self-consistent procedure is the calculation of charge density. The charge density spherically averaged inside the atomic sphere is given by the relation

$$\rho_{RI}(r) = \frac{1}{4\pi} \int_{-\infty}^{E_F} [\varphi_{RI}(E, r)]^2 N_{RI}(E) dE \quad (3)$$

where  $\varphi_{RI}(E, r)$  is the radial wave function.  $N_{RI}$  is the  $l$ -projected density of states

$$N_{RI}(E) = -\frac{1}{\pi} \text{Im} G_{RI}^{00}(E). \quad (4)$$

Writing  $\varphi_{RI}(E, r)$  in the form of the Taylor series and truncating after the first term, one can obtain the expression for the charge density in terms of density of states (DOS) moments [17]:

$$\rho_{RI}(r) = \frac{1}{4\pi} [\varphi_{RI}^2(r) m_{RI}^{(0)} + 2\varphi_{RI}(r) \varphi_{RI}'(r) m_{RI}^{(1)}] + \{\varphi_{RI}^2(r) - 2\varphi_{RI}(r) \varphi_{RI}'(r) \rho_{RI}^{\alpha} - \varphi_{RI}^2(r) \rho_{RI}^2\} m_{RI}^2 \quad (5)$$

where the DOS moments  $m_{RI}^{(q)}$  are given by the relation

$$m_{RI}^{(q)} = \int_{-\infty}^{E_F} [(E - E_{\nu RI})]^{(q)} N_{RI}(E) dE. \quad (6)$$

Such an approach can be readily used for impurity electronic-structure calculations in real space. First the DOS, potential parameters, potentials and the position of the Fermi level are calculated for a pure host solid. No crystal symmetry restrictions are required by the difference from the band-structure methods. Then an impurity is introduced, and the impurity potential, together with the potential of the neighbouring atoms, is calculated in a self-consistent way. All other atomic potentials are kept unchanged as in the host. The Fermi level is accepted to be the same as that of the host. To take into account the screening of the impurity potential we have used the charge-neutrality condition. The radii of the atomic impurity sphere and the spheres of its neighbours were fitted during iterations to maintain their charge neutrality. In this case redistribution of the charge density of the surrounding crystal is simulated by the appearance of charge density in the spherical layer between the initial and changed radii, which can be considered as the variant of the screening. This method is correct when the impurity sphere radius is close to that of the host, which is the case for the boron impurity in iron. A detailed description of this screening method is given in [22].

The potential of the pure BCC iron matrix was calculated by the TB-LMTO-REC method. The cubic cluster considered consisted of 896 atoms. 11, 15 and 30 pairs of recursion coefficients were calculated for s, p and d orbitals, respectively. The terminator proposed by Beer and Pettifor [23] was used. The atomic sphere radius of 2.661 a.u. has been accepted in the calculations. The magnetic-moment value for iron atoms obtained in our real-space LMTO-TB-REC calculations was  $2.20\mu_B$ , which coincided with those obtained by the reciprocal-space LMTO method, and showed the accuracy of our computational procedure to be sufficient.

We have made calculations for the boron impurity in BCC iron first in the scope of the single-site approximation. The first, second, third and fourth nearest-neighbour shells have been consecutively included in the self-consistent procedure. In all cases, s, p and d

orbitals of the boron atom were included in the basis; 10, 15 and 28 levels of recursion were calculated. As in the case of pure iron, the calculated cluster size was 896 atoms, except for the calculations taking into account the third and fourth nearest-neighbour shells, when the cluster size was increased up to 2000 atoms in order to avoid possible surface effects.

In order to overcome the integration difficulties for the impurity DOS, which appear due to its singularity at the band edge, we have applied the complex plane integration method. In the absence of a band gap it can be implemented in the recursion method in the following way. First, we determine the asymptotic values of the recursion coefficients  $a_\infty$  and  $b_\infty$  making use of the procedure of Beer and Pettifor [23]. Then, the 'square-root' terminator in the complex energy plan  $z = E + i\epsilon$  is built as follows:

$$t(z) = \frac{z - a_\infty - \sqrt{(z - a_\infty)^2 - 4B_\infty}}{2B_\infty}. \quad (7)$$

After this the Green function can be represented in the following form [24]:

$$G^{00}(z) = \frac{q_{n-1}(z) - B_n^2 t(z) q_{n-2}(z)}{\rho_n(z) - B_n^2 t(z) \rho_{n-1}(z)}. \quad (8)$$

Here  $q_n(z)$  and  $\rho_n(z)$  are complex orthogonal polynomials. The DOS moments, which we need to construct the charge density, can be easily obtained by the direct contour integration of the Green function in the complex plane [25]:

$$m^{(q)} = \frac{-1}{\pi} \text{Im} \int (z - E_v)^q G^{00}(z) dz. \quad (9)$$

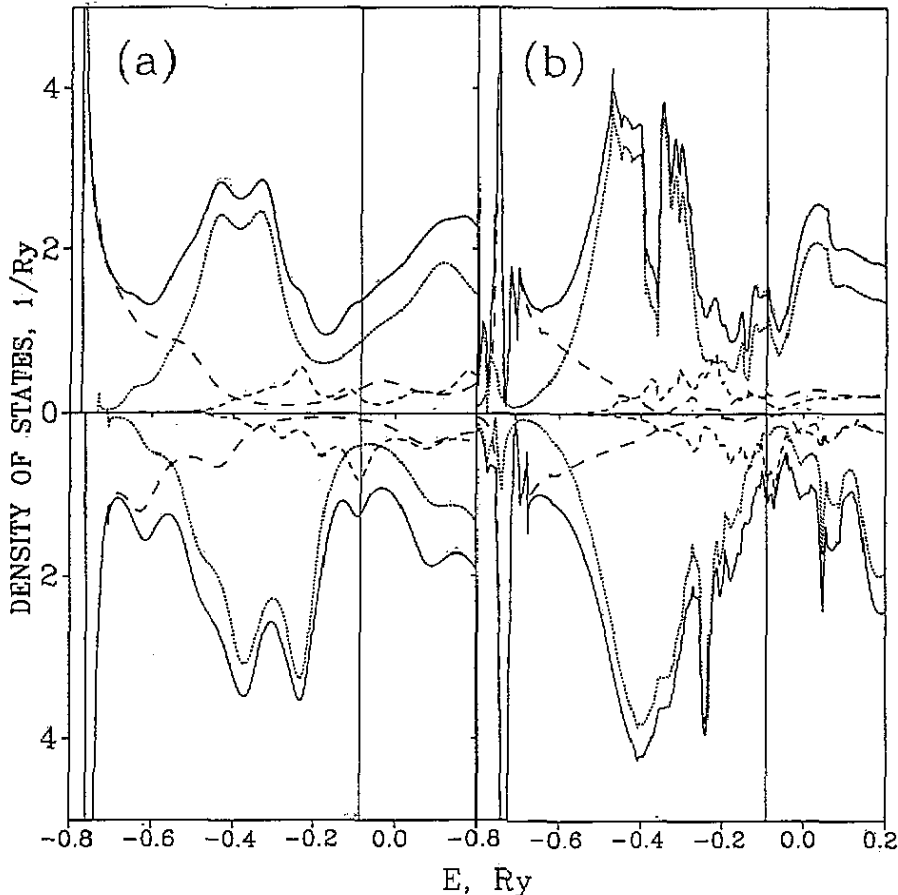
In the case when there is a gap in the density of states, instead of the square-root terminator, a more sophisticated terminator developed by Nex [24] should be used in the complex plane.

### 3. Results and discussion

The impurity's influence on the magnetic behaviour of iron in the iron-based dilute alloys is one of the interesting problems to be studied for such systems. Early theoretical investigations are only qualitative and are based on the estimation of the degree of hybridization of impurity centres with the host states. The calculations made within the scope of the embedded-cluster approach usually consider non-magnetic matrices, or in the magnetic case [10], the influence of the impurity on the magnetic behaviour of the matrix is not considered at all. We have investigated first the electronic states of the impurity both in the single-site approximation, and with regard to the dependence on the number of nearest-neighbour shells included into the self-consistent calculation.

Some idea of the accuracy of the method used can be obtained from figure 1, where the total and orbital-projected DOSs for the boron impurity in BCC iron are presented as calculated using the TB-LMTO-REC method in the single-site approximation and the single-site LMTO-GF method. The Green function matrix has been calculated using the analytical tetrahedron method [26] with 59  $k$  points in the irreducible part of the Brillouin zone. In both cases, impurity sphere radii were adjusted during the iterations in order to maintain the electroneutrality of impurities: they appeared to be 2.448 a.u. in the LMTO-GF calculation, and 2.420 a.u. in the TB-LMTO-REC calculation. The smaller value in the latter case may be due to the screened basis used, the wave functions of which are more localized. The

recursion method does not allow us to reproduce the fine structure of the density of states, but the main features are described well. This is obvious from a comparison with more precise results obtained by the LMTO-GF method. The boron density of states consists mainly of s orbitals, which are localized in energy near the band bottom and form the sharp resonance peak, and of the p states forming the double-peak structure in the middle of the band. The contribution of d states is small, but they are responsible for the small spin-down peak near the Fermi energy. The local magnetic moment at the boron atom is  $0.22\mu_B$  as calculated by the LMTO-GF method and  $0.23\mu_B$  by the TB-LMTO-REC method.



**Figure 1.** LDOS of boron impurity in BCC iron for both spin projections (solid line) and PDOS for s (short-dashed line), p (dotted line) and d (long-dashed line) states, calculated in the single-site approximation by the TB-LMTO-REC method (a) and the LMTO-GF method (b).

The impurity influences significantly the shape of the local density of states (LDOS) for the first shell of atoms, but at the same time the impurity potential causes definite oscillations of charge density in the adjacent spheres, resulting in the oscillations of magnetic moments of the atoms in different coordinational spheres (table 1). As is obvious from these data, the calculations taking into account one or two nearest-neighbour shells are not sufficient for an adequate description of the magnetic states of the whole system: the perturbation induced

by the impurity is not screened completely. Local magnetic moments for boron and iron atoms of the first shell appear to be too low. An increase of the number of neighbour shells included in the self-consistency from three to four gives a small change both in the magnetic moment of the impurity and its first neighbour, and in the DOS. This demonstrates that it is sufficient to include four neighbour shells in the self-consistent calculation to describe the interaction of the impurity with its first-neighbour shell. But the oscillations of the potentials of iron atoms from second-, third- and fourth-neighbour shells are still not sufficiently screened, as is seen from the values of their local magnetic moments. In band-structure methods, a qualitative analysis of impurity screening can be made by means of calculations of the change  $\Delta N(E_F)$  of integrated density of states of the whole crystal and the change  $\Delta M$  of total magnetization using a generalization of the Friedel sum rule given by Lloyd [27] and Lehman [28]. Unfortunately, this cannot be directly used in our calculations, because the recursion method is essentially local and operates only with the diagonal single-site Green function, so we are restricted to considering only local properties of the system, i.e. LDOS and local magnetic moments.

**Table 1.** Dependence of local magnetic moments of boron atom and iron atoms from different shells of neighbours on the number of shells included in the self-consistent calculations.

Number of shells	Local magnetic moment ( $\mu_B$ )				
	B	Fe1	Fe2	Fe3	Fe4
0	0.23	—	—	—	—
1	0.15	-0.91	—	—	—
2	0.18	-1.48	-1.65	—	—
3	0.21	-2.11	-1.78	-1.83	—
4	0.22	-2.17	-1.89	-1.91	-1.89

Figure 2 shows the total and partial densities of states (PDOS) for the boron impurity in BCC iron as calculated taking into account four neighbour shells, the LDOS for iron atoms from the first coordination shell and the DOS for pure iron. Hybridization of the resonance boron states with iron s states results in the formation of the peak located at the band bottom for the iron atoms from the first shell, and, to a lesser degree, for the iron atoms from the second shell of impurity neighbours. Boron p states are hybridized with metal d states over the whole band width. The shape of the p-type PDOS is changed for the first shell iron atoms: 1 and 1' features (figure 2) corresponding to the boron atom appear due to hybridization with its orbitals (p-p-type hybridization). Boron impurities produce small changes of iron d states: additional peaks 2 and 2' appear in the DOS for the first-shell atoms, which are caused by iron d-boron d hybridization. The latter, located at the Fermi level, shows that boron d states might be important to take into account when investigating kinetic properties of such systems (electro- and thermal conductivity, magnetic susceptibility etc). It is worth noting that no 2' peak in boron LDOS, or in iron LDOS, appears at the Fermi level when we take into account only one or two shells of neighbours in the calculations. This demonstrates the importance of proper self-consistent consideration of the impurity surroundings in quantitative calculations of dilute alloy properties.

Thus, the calculations performed show that the boron atom reveals sufficiently strong hybridization of its p and d states with iron p and d states, therefore the presence of boron impurities will not cause considerable changes in the strength characteristics of the system. However, there is weak s-d hybridization, and this defines the magnetic behaviour of the system under consideration. The local magnetic moment at the boron atom has the opposite

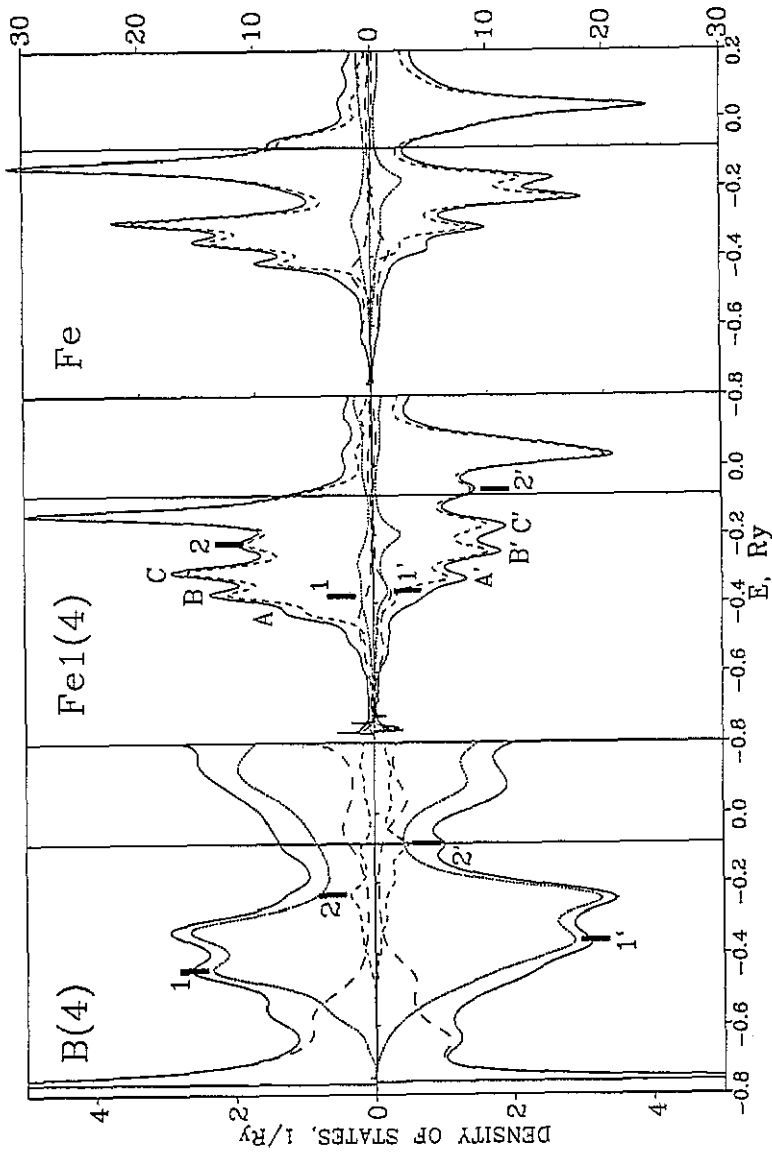


Figure 2. LDOS of the boron impurity in bcc iron calculated taking into account four nearest-neighbour shells, an iron atom from the first shell and an iron atom in the pure bcc crystal.



direction to the magnetization of the host crystal, which agrees with the conclusions in [2] on possible effects of s-d hybridization. In our case, s-d hybridization is relatively weak, and antibonding states near the Fermi level are almost vacant, whereas the bonding ones determine the negative magnetization, which is not very high. Due to weak s-d hybridization the local magnetic moment of boron calculated with four neighbour shells is rather close to that obtained in single-site calculations, and the magnetic moments of the iron atom do not differ much from those in pure iron. The strong p-d hybridization observed in the system also leads to negative magnetization: the antibonding p states of iron near the Fermi level are practically vacant, as they are located higher in energy than iron s states.

For quantitative evaluation of the influence of the boron impurity on the stability of the magnetic structure of the host, the calculations for the effective exchange interaction parameter  $J_0$  were carried out for nearest iron atoms. We have used the following expression for  $J_0$  [29, 30]:

$$J_0 = -\frac{1}{4\pi} \int_{-\infty}^{E_F} dE \operatorname{Im} Sp_L [\Delta_0 (T_{0\uparrow}^{00} - T_{0\downarrow}^{00}) + \Delta_0 T_{0\uparrow}^{00} \Delta_0 T_{0\downarrow}^{00}]. \quad (10)$$

Here  $\Delta_0 = p_{0\uparrow} - p_{0\downarrow}$ ,  $p$  is the potential function and  $\mathbf{T}$  the single-site scattering matrix

$$T_{LL}^{00}(E) = \frac{E - V_L}{\Gamma_L^{1/2}} G_{LL}^{00}(E) \frac{E - V_L}{\Gamma_L^{1/2}} - \frac{E - V_L}{\Gamma_L} \quad (11)$$

where  $V$  and  $\Gamma$  are potential parameters and  $G^{00}$  is the single-site Green function, which in the recursion method is represented in the continued fraction form. The increase or decrease of  $J_0$  in comparison with that in pure iron indicates the increase or decrease of stability of magnetic moment with respect to rotation [22, 30, 31]. The band-structure computational procedure for calculations of  $J_0$  in accordance with the approach of [29] and [30] has also been used for studying the stability of magnetic ordering for BCC and FCC iron [31]; the result obtained for BCC iron by the TB-LMTO-REC method (see table 2) is in reasonable agreement with results of band-structure calculations [31]. The difference is probably due to using the TB representation for the  $\mathbf{G}$  matrix in the case of the real-space calculations and different precision in the  $\mathbf{G}$ -matrix calculations by real- and reciprocal-space methods. It can be derived from the calculated values of  $J_0$  for the four nearest-neighbour iron atoms (table 2), that the boron impurity causes a small decrease of exchange parameters and magnetic moment only for the iron atoms in the first-neighbour shell. However, this decrease is insignificant (7%), allowing us to conclude, that the boron impurity does not influence the stability of the magnetic moment in BCC iron. Thus, an isolated impurity atom of boron only weakly influences the magnetic properties of iron atoms even from the first-nearest-neighbour shell. This is the consequence of a weak s-d and a strong p-d hybridization. One may expect that the magnetic behaviour of iron-boron alloys with a small content of boron will be determined completely by the iron matrix and the single-site approximation will work well in a study of magnetism in these systems.

Table 2. Exchange-interaction parameters for BCC iron and iron atoms from four nearest-neighbour shells of the boron atom in mRyd.

Sphere	Fe	1	2	3	4
$J_0$	18.0	16.7	18.1	18.0	18.0

#### 4. Conclusions

The TB-LMTO-REC calculations performed for a boron impurity in BCC iron lead to the conclusion that the weak hybridization of boron s states with iron d states along with the hybridization of boron p states with iron d states results in the situation when the impurity atom has a rather weak influence on the magnetic characteristics of iron atoms even from the first coordinational sphere of the impurity, so the magnetic behaviour of dilute iron-boron alloys with small boron content is completely determined by the iron matrix, and the single-site approximation is well justified for the study of such magnetic systems. At the same time, in quantitative investigations of kinetic properties, consideration of potential perturbations in not less than four nearest-neighbour shells appears to be necessary. The developed generalization of the real-space TB-LMTO-REC method for impurity calculations is precise enough for studying magnetic interactions and electronic structure of the sp impurities (such as boron) in metals with stable magnetic structure (such as BCC iron). Calculations of the magnetic interactions of the boron impurities for other structural modifications of the iron (especially for FCC and amorphous iron with respect to the asymptotical behaviour of amorphous iron-boron alloys) will be the subject of a further publication.

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#### References

- [1] Koenig C, Leonard P and Daniel E 1981 *J. Physique* **42** 1015
- [2] Akai H, Akai M, Blugel S, Zeller R and Dederichs P H 1984 *J. Magn. Magn. Mater.* **45** 291
- [3] Akai M, Akai H and Kanamori J 1985 *J. Phys. Soc. Japan* **54** 4246
- [4] Chaki T K 1990 *Phil. Mag. Lett.* **61** 5
- [5] Samsonov B V, Markovskii L P, Zhigach A F and Valyashko M G 1960 *Boron in Compounds and Alloys* (Kiev: Ukrainian Academy Nauk) (in Russian)
- [6] Perkins R S and Brown 1972 *J. Phys. F: Met. Phys.* **5** 906
- [7] Brown P J and Cox J L 1971 *Phil. Mag.* **23** 705
- [8] Zeller R and Dederichs P H 1979 *Phys. Rev. Lett.* **42** 1713
- [9] Podloucky R, Zeller R and Dederichs P H 1980 *Phys. Rev. B* **33** 5777
- [10] Koenig C and Daniel E 1981 *J. Physique Lett.* **42** L193
- [11] Gunnarsson O, Jepsen O and Andersen O K 1983 *Phys. Rev. B* **27** 7144
- [12] Braspenning P J, Zeller R, Lodder A and Dederichs P H 1984 *Phys. Rev. B* **29** 703
- [13] Stefanou N, Oswald A, Zeller R and Dederichs P H 1987 *Phys. Rev. B* **35** 6911
- [14] Drittler B, Stefanou N, Blugel S, Zeller R and Dederichs P H 1989 *Phys. Rev. B* **40** 8203
- [15] Kemdradt U, Drittler B, Hoshino T, Zeller R and Dederichs P H 1991 *Phys. Rev. B* **43** 9487
- [16] Kontsevoi O Yu, Mryasov O N and Gubanov V A 1992 *Fiz. Tverd. Tela* **34** 2624; 1992 *Bull. Am. Phys. Soc.* **37** 288
- [17] Nowak H J, Andersen O K, Fujiwara T, Jepsen O and Vargas P 1991 *Phys. Rev. B* **44** 3577
- [18] Haydock R 1980 *Solid State Physics* vol 35, ed H Ehrenreich, F Seitz and D Turnbull (New York: Academic)
- [19] Andersen O K and Jepsen O 1984 *Phys. Rev. Lett.* **53** 2571

- [20] Andersen O K, Jepsen O and Glotzel D 1985 *Highlights of Condensed Matter Theory* ed F Bassani, F Fumi and M Tosi (Amsterdam: North-Holland) p 59
- [21] Barth U and Hedin L 1972 *J. Phys. C: Solid State Phys.* **5** 1629
- [22] Anisimov V N, Antropov V P, Gubanov V A, Ivanovsky A L, Kurmaev E Z, Liechtenstein A I and Postnikov A V 1989 *Electronic Structure of Impurities and Defects in Transition Metals, their Alloys and Compounds* (Moscow: Nauka)
- [23] Beer N and Pettifor D G 1984 *Electronic Structure of Complex Systems* ed P Phariseau and W M Temmerman (New York: Plenum) p 769
- [24] Nex C M M 1984 *Comput. Phys. Commun.* **34** 101
- [25] Zeller R, Deutz J and Dederichs P H 1982 *Solid State Commun.* **44** 993
- [26] Lehman G and Taut M 1972 *Phys. Status Solidi b* **54** 469
- [27] Lloyd P 1967 *Proc. Phys. Soc.* **90** 207
- [28] Lehman G 1975 *Phys. Status Solidi b* **70** 737
- [29] Liechtenstein A I, Katsnelson M I and Gubanov V A 1984 *J. Phys. F: Met. Phys.* **14** L125
- [30] Liechtenstein A I, Katsnelson M I and Gubanov V A 1985 *Solid State Commun.* **54** 327
- [31] Mryasov O N, Liechtenstein A I and Gubanov V A 1992 *Phys. Rev. B* **45** 12330