Total energy and magnetic moments in disordered Fe_xCu_{1-x} alloys

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Magnetic states of fcc disordered substitutional alloys Fe_xCu_{1-x} have been studied by the Korringa-Kohn-Rostoker method within the coherent-potential approximation. Total-energy calculations with the fixed-spin-moment procedure have been used to investigate the behavior of magnetic phases with an increasing concentration of Cu. These investigations are restricted to ferromagnetic states. The magnetic ground state of the alloy is highly sensitive to the equilibrium volume of the unit cell. Fe_xCu_{1-x} is nonmagnetic at the equilibrium lattice constant up to a Cu concentration of 18%. It discontinuously transforms into a high-spin state with a moment of about $2\mu_B$ per cell for larger concentrations. The local Fe moment is calculated to be $2.70\mu_B$ in Cu and $2.52\mu_B$ in fcc Fe. In the nonmagnetic region the lattice constant increases and the bulk modulus decreases with Cu concentration while in the magnetic phase both do not depend on the concentration and coincide well with those of pure Cu. [S0163-1829(98)01506-9]

I. INTRODUCTION

The bulk miscibility of Cu in both γ (fcc) and α (bcc) Fe is very small, only a few percent at higher temperatures. Also the solubility of Fe in bulk Cu is very low.[1,2] Nevertheless the Fe_xCu_{1-x} alloy is interesting to investigate for several reasons: (i) There is experimental evidence that during the epitaxial growth of Fe on Cu(001) intermixing at the interface occurs (cf. Refs. 3 and 4); (ii) metastable Fe_xCu_{1-x}alloys can be prepared experimentally in a wide range of concentrations (cf. Refs. 5–7); (iii) the electronic and magnetic properties of Fe_xCu_{1-x} to date have not been investigated in detail. Ultrathin films of Fe grown on fcc surfaces have been extensively investigated to study the magnetic properties of γ-Fe. Fe grows on Cu(001) pseudomorphically, because a small negative misfit of about 1% forces only a slightly increased lattice spacing of Fe and a small tetragonal distortion. Low-energy electron diffraction has shown that the deposited Fe should have a fcc structure on the Cu substrate for a coverage up to 10–14 monolayers (ML).[8] The addition of more Fe leads to a martensitic phase transition and the overlayer reverts the structure to bcc.[9] Detailed experimental investigations of the Fe/Cu(001) system have shown that the magnetic properties of the Fe films depend strongly on the preparation conditions. Giergiel *et al.*[10] have studied the growth and morphology of ultrathin Fe films on Cu(001) by means of the scanning tunnelling microscope (STM). They have prepared films at low temperature (LT) (130 K) which were subsequently annealed to 300 K before imaging. Secondly, they have prepared room temperature (RT) deposited films. The magnetic properties of such films have been reported by Thomassen *et al.*[11] (RT) and Allenspach and Bischof[12] (LT). The films show two common characteristics: (i) lack of magnetic ordering below 2 ML, (ii) perpendicular anisotropy in the 2–5 ML thickness range. Above 5 ML the properties of the films differ (cf. Refs. 11–13). Giergiel *et al.*[10] have discussed the delayed onset of ferromagnetic ordering in terms of some kind of magnetic percolation. One reason for the delayed onset of the ferromagnetic order could be an intermixture at the Fe-Cu interface. Such processes have been reported in RT-deposited films.[3,4] A detailed study of the magnetic properties of Fe_xCu_{1-x} bulk alloys could help to test the importance of intermixing for the delayed onset of ferromagnetism in such films. The fcc structure of Fe can also be stabilized in the form of precipitates in a Cu matrix. Neutron scattering experiments have shown an antiferromagnetic (AF) state[14] or a AF structure modulated with a spiral-density wave component.[15] However, the ferromagnetic (FM) structure was also found in Mössbauer[16] and susceptibility measurements.[17]

Although the miscibility of Fe in Cu and Cu in Fe is very small, several methods to produce metastable solid solutions such as vapor quenching,[5] vapor deposition[6] and ion beam mixing[18] are known. It has been known for a long time that metastable solid solutions of Cu with concentrations up to 6.5% Fe can be prepared by splat-cooling of the melt.[19] Fe_xCu_{1-x} alloys can be prepared also by mechanical alloying.[20–23] The Fe_xCu_{1-x}alloy shows a single bcc phase on the Fe rich side and a single fcc phase on the Cu rich side. The phase boundaries to the coexistence region of fcc and bcc phase depend on the method of preparation. The coexistence region is given to be $0.6 \leqslant x \leqslant 0.8$ by Eckert *et al.*[21] (mechanical alloying) and $0.4 \leqslant x \leqslant 0.6$ by Sumiyama *et al.*[5] (thermal evaporation). Extended x-ray-absorption fine structure studies recently published have shown that ball milled Cu and Fe really undergo true alloying on the atomic level.[24]

The magnetic phase transitions in 3*d* metals are investi-

gated by Moruzzi *et al.*[25–27] It has been shown[25] that different types of transitions can occur. The calculated magnetic moment and total energy dependent on the Wigner-Seitz radius r_{WS} for bcc iron show a second-order transition from a nonmagnetic (NM) to a ferromagnetic (FM) state. The behavior for pure fcc iron is much more complicated. A nonmagnetic state is obtained for r_{WS} less than or equal to the equilibrium value of 2.54 a.u. Antiferromagnetic ordering is most favorable up to $r_{WS}=2.71$ a.u.[26] Larger values of r_{WS} lead to a high-spin FM state. In a tiny range of volumes also a low-spin FM solution exists, which has higher energy than the AF structure. The *ab initio* disordered local moment method[28] is also used to calculate the temperature and volume dependence of the magnetic moment and the spin-spin correlations of γ-Fe.[29] In a recent paper also antiferrimagnetic solutions are discussed.[30] According to the experiments of Tsunoda,[15] the ground state of γ-Fe is a noncollinear magnetic state. Calculations of Sandratskii and co-workers[31] for spiral states have demonstrated that the minimum of the total energy of γ-Fe is obtained for a wave vector of $\mathbf{q}_m=(0,0,0.6)\ \ 2\pi/a$.

For the nonmagnetic metals like V the phase transitions from the nonmagnetic to a magnetic state occur at volumes which cannot be reached experimentally. Binary substitutional alloys have one additional external parameter, i.e., the concentration of the components. Variation of the concentration changes the effective number of valence electrons per cell and thus shifts the Fermi energy with respect to the position of the *d* bands. This may lead to a situation where the Stoner criterion is satisfied and a magnetic phase transition can occur at normal pressure. To investigate the type of the phase transition it is necessary to calculate magnetic binding surfaces, i.e., constant energy contours in the magnetization-versus-volume plane, for different concentrations. Such calculations have been published recently for the Invar alloy Fe_xNi_{1-x} for concentrations close to the critical concentration $x=0.65$.[32–35] A first-order phase transition from the NM to FM state is found in Ref. 35 for $x\approx 0.65-0.70$ by means of the coherent-potential approximation within the Korringa-Kohn-Rostoker band structure scheme based on the local spin density approximation (KKR-CPA LSDA).

The ferromagnetism in ordered FeCu metastable alloys was previously investigated by Serena and García[36] by means of the linearized augmented-plane-wave method (LAPW). They have calculated paramagnetic densities of states for a series of ordered intermetallic compounds at a fixed lattice constant, which was that of fcc Cu for fcc compounds and that of α-Fe for the same intermetallic compounds with bcc structure. Magnetism was discussed in terms of the Stoner theory.[37,38]

In this paper we present calculations of the magnetic binding surfaces for fcc Fe_xCu_{1-x}. The KKR-CPA method is used. We investigated the phase transitions as a function of the concentration x. Magnetovolume instabilities, and the dependence of lattice constant and bulk modulus on the concentration as well as mixing enthalpy are discussed in detail.

II. DETAILS OF THE KKR-CPA CALCULATIONS

The self-consistent-field (SCF) spin-polarized KKR-CPA method together with the fixed spin moment procedure[39,40] is used for the calculation of the total energy of binary substitutional fcc Fe_xCu_{1-x} alloys. The electron charge density and the crystal potential are assumed to be spherically symmetrical in muffin-tin (MT) spheres and constant in the interstitial region. Results, calculated in the atomic sphere approximation (ASA), where the Wigner-Seitz cell is replaced by an atomic sphere of the same volume, are given for comparison. For the exchange and correlation potential the formulation of von Barth and Hedin[41] modified by Janak[42] is used and *s*, *p*, *d*, and *f* valence states are taken into account. All calculations are performed nonrelativistically with core relaxation at each iteration during the SCF cycle. A rectangular contour in the complex energy plane is used for the energy integration. The tetrahedron integration technique with a subsequent subdivision of tetrahedra, whenever the phase of the integrand cannot be linearly interpolated, is applied for the Brillouin-zone integration for energy points close to the real axis.[43,44] Different methods of the solution of the CPA equation are used along the complex energy contour. For energies far away from the real axis the CPA solution is found by 1–2 iterations starting from the average *t* matrix. Close to the Fermi energy the starting value for the coherent scattering matrix $t_c(E)$ is constructed by extrapolating $t_c(E)$ along this part of the energy contour. Only 1–2 iterations are required for the solution of the CPA equation for this part of contour. For the self-consistency iterations the Broyden acceleration procedure is used.[45] Convergence is considered to be achieved if the root-mean-square (rms) difference of input $\varrho_{in}(r)$ and output $\varrho_{out}(r)$ charge densities is less than 10^{-4}. The rms error in the total energy, fitted to a third order Birch function,[46] is less then 0.1 mRy in this case.

III. DISCUSSION

We start our discussion with pure fcc iron. By means of the fixed-spin-moment procedure the magnetic and structural binding surfaces are investigated. Some of the results are presented in Fig. 1(a). We obtain $r_{WS}=2.53$ a.u. for the equilibrium lattice constant of γ-Fe. In Fig. 1(a) the total energy as a function of the magnetic moment is plotted for r_{WS} values near the equilibrium value of Cu for which we obtain $r_{WS}=2.64$ a.u. The total energy of γ-Fe at the Cu lattice constant is more than 10 mRy higher than the ground state value at $r_{WS}=2.53$ a.u. Figure 1(a) shows that the transition to the high-spin ferromagnetic ground state with a moment of $2.5\mu_B$ occurs between $r_{WS}=2.64$ a.u. and $r_{WS}=2.65$ a.u.

Figure 2(a) shows the dependence of the total energy and the magnetic moment on the Wigner-Seitz radius for γ-Fe. A nonmagnetic (NM), a low spin ferromagnetic (LSF), and a high-spin ferromagnetic state (HSF) are obtained. Small regions of coexistence of the different phases exist. We have investigated only ferromagnetic states of the Fe_xCu_{1-x} alloys, so antiferromagnetic and noncollinear states are not considered. Our results coincide with previous calculations.[26,30,47] The second LSF state was found in the calculation of Zhou *et al.*[30] and Kübler[47] but not by Moruzzi *et al.*[26,48] We found no indication of this LSF state in our calculations. If only collinear arrangements of the moments are allowed, the ground state of γ-Fe will be antiferromag-

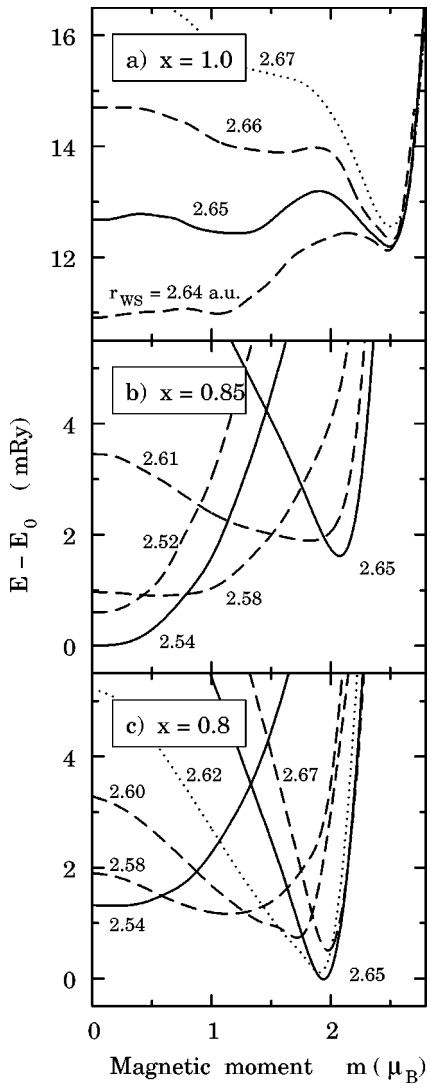

FIG. 1. Total energy (calculated in MT approximation) dependent on the average magnetic moment per atom for fcc Fe_xCu_{1-x} at several values of the Wigner-Seitz radius. The total energy is related to the ground state energy E_0. The equilibrium volume of Cu corresponds to $r_{WS}=2.64$ a.u. Different concentrations are considered: (a) $x=1$, pure γ-Fe; (b) $x=0.85$; (c) $x=0.8$.

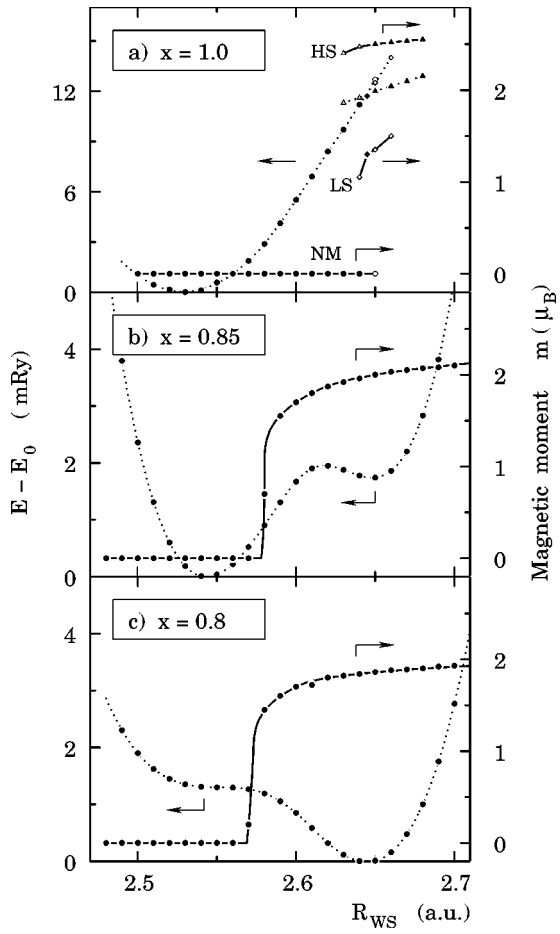

FIG. 2. The total energy (dotted lines) and the average magnetic moment per atom (solid lines) calculated in the MT approximation for fcc Fe_xCu_{1-x} for different values of the Cu content: (a) $x=1$, pure γ-Fe; (b) $x=0.85$; (c) $x=0.80$. In (a) the total energy and the magnetic moments of the different magnetic states are marked by the same symbols (triangles – HS state, diamond – LS state, circle – nonmagnetic state). Full symbols correspond to the ground state solution, the open ones to metastable states. For other concentrations (b),(c) only one stable solution is obtained marked by circles.

netic for 2.54 a.u.$\leqslant r_{WS}\leqslant$2.71 a.u. A noncollinear magnetic structure with a spiral wave vector $\mathbf{q}_m=(0,0,0.6)\ 2\pi/a$ will decrease the energy and presumably presents the true ground state.[31] However, if only ferromagnetic states are considered γ-Fe undergoes two consecutive first-order phase transitions (NM $\rightarrow$ LSF, LSF $\rightarrow$ HSF).

If Cu is added to form the alloy it can be seen [cf. Figs. 1(b) and 1(c)] that the equilibrium lattice constant increases. In MT approximation the first order phase transition occurs at $x=0.82$ and the equilibrium lattice constant of the alloy discontinuously jumps to about the lattice constant of pure Cu [see Fig. 5(b)]. The phase transition is connected with a change in the magnetic properties. $Fe_{0.85}Cu_{0.15}$ has an equilibrium value of $r_{WS}=2.54$ a.u. and the local minimum in $E_{tot}=E(r_{WS})$ at 2.65 a.u. is about 1.8 mRy higher in energy, i.e., the ground state is nonmagnetic. However, for $x=0.8$ the alloy is stable at the Cu lattice constant and has an average magnetic moment per atom of $1.85\mu_B$. The phase transition is characterized by magnetovolume instabilities. In the high-spin state the Fe atoms have, due to magnetovolume expansion, a volume similar to the value of Cu, i.e., $r_{WS}=2.65$ a.u., while the energy minimum of the nonmagnetic state occurs at about 2.54 a.u. Figure 2 shows that the LSF state is sensitive to the Cu concentration and a change in the type of the phase transition occurs. At the concentration $x=0.82$ a first-order phase transition from nonmagnetic to ferromagnetic state takes place. In ASA approach the critical concentration is $x=0.77$. The difference of 5% indicates the uncertainty in our calculation arising from the approximate treatment of the charge density and its potential. Since the phase transition at $x\cong 0.8$ is quite analogous to the transition of the Invar system $Fe_{0.35}Ni_{0.65}$ we expect the $Fe_{0.2}Cu_{0.8}$ alloy to show Invar properties at elevated temperatures as well.

The calculation of FeCu alloys by Serena and García[36] is based on the LAPW method. They have calculated the paramagnetic densities of states for intermediate fcc intermetallic compounds at the equilibrium Cu lattice constant. A Stoner model is used to investigate the spin polarization of these

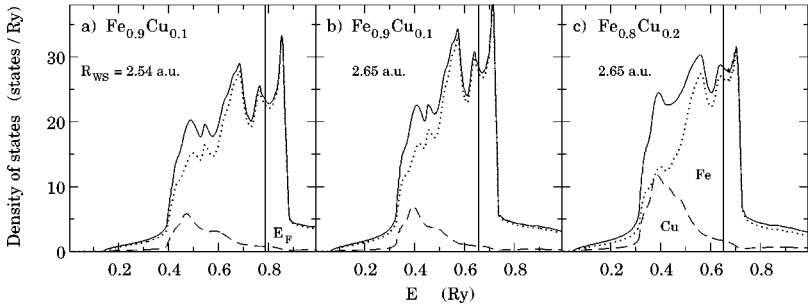

FIG. 3. Comparison of the paramagnetic densities of states (calculated in MT approximation) for different WS radii and concentrations: (a) $Fe_{0.9}Cu_{0.1}$, $r_{WS}=2.54$ a.u.; (b) $Fe_{0.9}Cu_{0.1}$, $r_{WS}=2.65$ a.u.; (c) $Fe_{0.8}Cu_{0.2}$, $r_{WS}=2.65$ a.u.

compounds. At fixed Cu lattice constant they found $Fe_{0.5}Cu_{0.5}$ magnetic, but $Fe_{0.25}Cu_{0.75}$ nonmagnetic. For $Fe_{0.75}Cu_{0.25}$ they predicted a magnetic moment per Fe atom of $2.3\mu_B$ by means of the Stoner theory. They also performed a LAPW-LSDA calculation for $Fe_{0.75}Cu_{0.25}$. This calculation gives an equilibrium lattice constant which is less than that of Cu and a magnetic moment of $1.85\mu_B$ per Fe atom. Otherwise, they obtained a magnetic moment of $2.3\mu_B$ for the Cu lattice constant, a result which corresponds to the prediction of the Stoner theory.

If we compare the results of the ordered structures with our results we find that the magnetic moment is comparable but our equilibrium lattice constant for $x=0.75$ is higher (6.76 a.u. compared with 6.62 a.u. in Ref. 36).

To investigate the effects near the phase transition from the paramagnetic state to the high-spin ferromagnetic state between $x=0.9$ and $x=0.8$ we have calculated the densities of states (paramagnetic and spin polarized) for these concentrations and different WS radii. The results are given in Figs. 3 and 4. Two concurrent processes can be inferred from the paramagnetic density of states (DOS) given in Fig. 3. The increase of the WS radius for $Fe_{0.9}Cu_{0.1}$ leads to a band narrowing of the partial Fe-DOS and an increase of the DOS at the Fermi energy $n(E_F)$. This leads to an average magnetic moment of about $2.25\mu_B$ for the metastable state. If we fix r_{WS} at 2.65 a.u. and further increase the Cu content by 10%, the DOS of $Fe_{0.8}Cu_{0.2}$ at the Fermi energy is only slightly changed, while the d character at E_F as given by the partial Fe-DOS in Fig. 3 slightly decreases. On the other hand, the effective Fe band further narrowed and the local DOS of an Fe atom, which unlike the partial DOS is not weighted by the Fe concentration, substantially increases. As a result the ferromagnetic state is stabilized. Due to the filled majority band the local Fe moment is practically unchanged ($2.5\mu_B$), while in accordance with the simple dilution model the average moment decreases to $1.97\mu_B$.

Figure 4 shows the spin-polarized densities of states for $Fe_{0.8}Cu_{0.2}$ at $r_{WS}=2.65$ a.u. The equilibrium state with a moment of $1.97\mu_B$ is given in Fig. 4(b). The two other states are calculated with the fixed-spin-moment method. They are higher in total energy [cf. Fig. 1(c)]. We have found in our calculations that configuration with the totally filled d bands of spin-up electrons corresponded to a local minimum in total energy. Figure 4 shows that the DOS of the minority electrons is considerably broader than the spin up part. This is a direct consequence of the energy separation for majority and minority states and is typical for all ferromagnets and ferromagnetic alloys.[33]

The results of our calculations for various properties of the Fe_xCu_{1-x} alloys, average magnetic moment per atom, lattice constant, bulk modulus and enthalpy of mixing, are summarized and compared with experimental results in Fig. 5. The first-order phase transition from the nonmagnetic to the ferromagnetic alloy at 18% of Cu leads to characteristic discontinuities in all quantities. Calculations within both the atomic sphere approximation and the MT approximation are presented. The MT approximation seems to give a somewhat better description of the crystal potential, leading to better results for the lattice parameter. The main difference between the two approximations is a shift in the phase transition to lower Cu concentrations if the MT approximation is used. Otherwise, the magnetic properties are not very sensitive to the approximations in the potential, except that the equilibrium lattice constant is more strongly influenced.

In Fig. 5(a) the magnetic moment per atom is compared with experimental data of Sumiyama *et al.*[5] obtained on sputtered samples. A characteristic deviation from a simple dilution law, upwards in the bcc region and downwards in

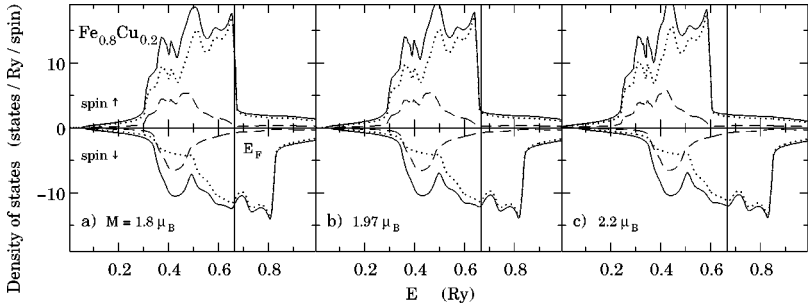

FIG. 4. Spin-polarized densities (calculated in MT approximation) of states for fcc $Fe_{0.8}Cu_{0.2}$ at $r_{WS}=2.65$ a.u. for different average magnetic moments: (a) $1.8\mu_B$; (b) $1.97\mu_B$; (c) $2.2\mu_B$.

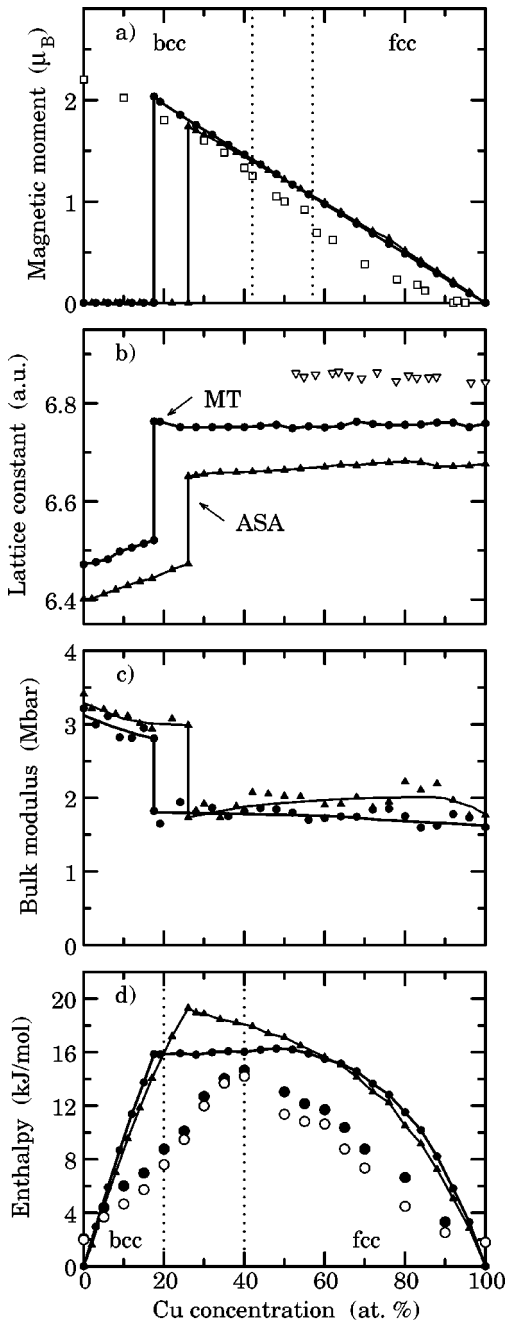

FIG. 5. Different quantities for fcc Fe_xCu_{1-x} dependent on the Cu concentration. Calculated results in MT approximation are marked by full circles and the atomic sphere approximation (ASA) is marked by triangles. (a) Magnetic moment per atom. Squares mark experimental values from sputtered alloys (Ref. 5). The dotted lines mark the coexistence region according to Ref. 5. (b) The equilibrium lattice constant dependent on the Cu concentration. ∇ – experimental values for sputtered alloys (Ref. 5). (c) Bulk modulus in dependence on the Cu concentration calculated within MT approximation and ASA. The lines represent a spline interpolation between the calculated values. (d) Concentration dependence of the mixing enthalpy for fcc Fe_xCu_{1-x}. The calculations are compared with experimental values obtained from powder samples prepared by means of mechanical alloying (Ref. 21). ● – maximum total stored enthalpy after 8 h of milling, ○ – residual total stored enthalpy after 24 h of milling.

the fcc region, exists in the experimental data. The alloy becomes nonmagnetic for a Cu content of 92%. Experimental results on mechanically alloyed samples[22] do not show deviations from a simple dilution behavior.

Our calculations, restricted to the fcc structure, show a simple dilution behavior with a slope of $-0.024\mu_B$ per at. % Cu which coincides with the value $-0.0225\mu_B$ per at. % Cu of Ma *et al.*[22] In the investigation of Ma *et al.* samples with an Fe content less than 10% are not investigated. Also the results of Chien *et al.*[6] show a simple dilution behavior, but no data for $x \leqslant 0.1$ are included. Therefore the magnetism of Fe_xCu_{1-x} alloys with a low Fe concentration is not totally clear. A spin-glass-like behavior, reported by Zibold and Korn,[49] was not found in later experimental investigations. Recent Mössbauer and magnetic measurements[7] indicate the superparamagnetic behavior in $Fe_{0.25}Cu_{0.75}$ mechanically alloyed. These experiments also show that the Fe atoms dissolved in the fcc Cu have a magnetic moment similar to that for the Fe in α phase.

In the low concentration limit case of a dilute alloy the CPA reduces to an impurity calculation in the single site approximation. The local magnetic moment of an Fe atom in Cu matrix in our calculations is $2.70\mu_B$. The KKR Green function calculations[50] and real-space linear muffin-tin orbital (LMTO) ASA calculations[51] are $2.51\mu_B$ and $2.69\mu_B$, respectively, which coincides with our result. Fe_xCu_{1-x} bulk alloys with dilute Fe concentrations form progressively ferromagnetic Fe clusters in the Cu matrix. By annealing, the coherently precipitated clusters grow much larger to behave as γ-Fe and the Fe atoms are aligned antiferromagnetically. The formation of precipitates or of a spin glass cannot be described within our KKR-CPA formalism.

Local moment disorder can be investigated using the KKR-CPA, as proposed by Pindor *et al.*[28] Calculations for CrFe, FeNi, and NiMn alloys have been recently done by Akai and Dederichs.[52] Additional degrees of freedom have been introduced for the magnetic components in this method, e.g., Fe atoms with moments up and down were averaged separately.

The lattice constant of the fcc Fe_xCu_{1-x} alloys given in Fig. 5(b) represents the magnetovolume instability at the magnetic phase transition. The equilibrium lattice constant of nonmagnetic fcc iron was approximately 4% less (in the MT calculations) than the pure Cu lattice constant. The equilibrium lattice constant of fcc Fe coincides with the results of Moruzzi *et al.*[26] and the calculated Cu lattice constant agrees with the value given by Moruzzi *et al.*[53] An increase of the lattice constant with Cu concentration is obtained in the Fe-rich alloys. The lattice constant for $x > 18\%$ corresponds practically to the lattice constant of pure Cu. Thus, in the high-spin state an Fe atom has about the same volume as a Cu atom, so that upon substitution the lattice constant is not changed. From this point of view sputtered Fe_xCu_{1-x} alloys could be lattice matched to a Cu substrate in a wide range of Fe concentrations. The experimental data of Sumiyama *et al.*[5] for sputtered samples at room temperature (on a polymidine substrate) are also given. The data also show the typical independence on the Cu concentration in the fcc region.

We have also calculated the bulk modulus for the alloys, using the calculated dependence of the total energy on the volume. The equation of state was found by fitting of the *ab*

initio results to the Birch equation[46] with $N=3$. The increase of the equilibrium lattice constant with Cu concentrations in the Fe-rich region corresponds with a decrease of the bulk modulus. For the magnetic alloys the bulk modulus is practically constant. The experimental value of the bulk modulus of Cu [1.37 Mbar (Ref. 54)] agrees with our calculated value of 1.6 Mbar.

An important starting point for the experimental investigation is the large positive enthalpy of mixing ($\Delta H_{mix} = +13$ kJ/mol for $Fe_{50}Cu_{50}$ according to Miedema's semiempirical model[55]). At the start of the experiment, the question was if metastable phases could be formed in such a system. The enthalpy of mixing was measured at mechanically alloyed samples by Eckert *et al.*[21] Experimental data are obtained by means of differential scanning calorimetry (DSC). Maximum values of 14 kJ/mol are obtained. The experimental data coincide well with Miedema's calculations and show that mechanical alloying can store enough enthalpy in the system to overcome the high positive enthalpy of mixing.

We have calculated the enthalpy of mixing ΔH_{mix} from the following relation:

$$\Delta H_{mix} = E_{\mathrm{FeCu}} - xE_{\mathrm{Fe}} - (1-x)E_{\mathrm{Cu}}. \tag{1}$$

E_{FeCu} is the equilibrium total energy of the alloy, whereas $E_{\mathrm{Fe(Cu)}}$ are the equilibrium total energies of pure Fe(Cu) and x is the concentration of the Fe atoms. The magnetic contribution to the total energy leads to a discontinuous slope in the enthalpy of mixing. Our values calculated *ab initio*, especially the maximum value for $Fe_{0.60}Cu_{0.40}$, coincide well with the experimental results.[21] The results of calculations using more approximate methods do not generally correspond better with the experimental results.[22,55]

IV. CONCLUSIONS

We have performed a systematic study of fcc Fe_xCu_{1-x}alloys by means of the KKR-CPA method. A first-order phase transition from the nonmagnetic to the ferromagnetic phase is obtained at about $x \cong 0.8$. The type of phase transition changes with increasing Cu concentration. In γ-Fe a LSF state exists, which disappears with increasing Cu content. In the critical concentration range these alloys should show Invar properties. For larger Cu concentrations ($0 < x < 0.8$) the lattice constant and the bulk modulus of the metastable Fe_xCu_{1-x} alloys are constant and practically equal to the values of pure Cu. Therefore a Cu substrate, widely used for investigations of γ-Fe, could be interesting as well for the preparation of Fe_xCu_{1-x} alloy systems, which could be produced by sputtering.

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