Ab initio investigation of the Invar anomaly in ordered fcc Fe-Pt alloys

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The magnetovolume anomaly in ordered fcc Fe-Pt Invar alloys is studied by *ab inito* Korringa-Kohn-Rostoker atomic-sphere approximation technique in the framework of density-functional theory. The paramagnetic state above the magnetic ordering transition temperature is treated using the disordered local moment (DLM) approach. We show that the DLM approach is able to describe and explain the Invar anomaly in ordered Fe-rich Fe-Pt alloys similarly to our previous work for the disordered modification. In particular, our calculations predict the weakening of the Invar anomaly in chemically ordered compositions as compared to the disordered case as well as a decreasing magnetovolume anomaly with increasing Pt concentrations for both ordered and disordered cases in full agreement with experimental observations. The detailed study of the Fe_3Pt compound with varying chemical long-range order has revealed a continuously decreasing spontaneous volume magnetostriction with increasing degree of order. This can be understood from the corresponding band structure of random and ordered alloys.

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I. INTRODUCTION

The anomalously low thermal expansion found in some magnetic materials below the magnetic critical temperature (Invar effect)[1,2] is the subject of persistent interest in solid-state physics for more than a century since its discovery by Guillaume in 1897.[3] The oldest known, studied, and technologically still most important Invar systems are fcc alloys of iron with other transition elements which are regarded as "classical"[2] Invar alloys. Among them the Fe-Pt alloys have attracted special interest since they are the only Fe-based Invar alloys existing both in a chemically ordered and disordered form.

The existence of ordered fcc Fe-Pt compounds has been regarded as a very strong argument against theories that attribute the Invar effect solely to chemically disordered systems. In general any theory which intends to provide a common picture of the Invar phenomena in magnetic materials has to explain the Invar effect in disordered and ordered Fe-Pt alloys on the same footing and reproduce the experimentally observed differences in their behavior. This means in particular the observed reduction of the spontaneous volume magnetostriction ω_{s0} in chemically ordered samples at a fixed alloy composition with respect to the disordered ones.[4] The quantity ω_{s0} is defined as the relative difference in the equilibrium volumes between for the $T=0$ K magnetic ground state and a reference paramagnetic state above the magnetic ordering temperature T_c.[1,2]

In this paper we calculate ω_{s0} in ordered, partially ordered, and random FePt alloys using the disordered local moment (DLM) approach for the paramagnetic state above the magnetic ordering temperature. This approach, as has recently been shown,[5] provides an adequate description of the Invar anomaly for disordered fcc and bcc Fe based alloys (fcc Fe-Pt, fcc Fe-Pd, bcc Fe-Co),[6] as well for pure hcp Gd metal,[7] which represents a system with well defined local atomic moments. The application of the *ab initio* DLM formalism to the Invar problem can be traced back to Johnson and co-workers,[8,9] where Fe-Ni Invar alloys have been considered.

It should be noticed that in contrast to Fe-Pt(Pd) alloys, the straightforward application of the DLM formalism to disordered magnetic states in Fe-Ni meets certain difficulties since Ni, being intrinsically magnetic, does not possess a stable local moment in the DLM state (see, e.g., Ref. 10). In this case it was advocated that *ab initio* DLM calculations should be combined with a treatment of the effects of the partial chemical ordering in Fe-Ni. The most recent development along these lines was followed by Crisan *et al.*[11] (see also the phenomenological treatment of chemical ordering in Fe-Ni by Lagarec *et al.*[12]). In this respect Fe-Pt alloys exhibit a completely different behavior, since there is no magnetic moment on the Pt atoms in the paramagnetic case (at least at temperatures close to ambient temperature), and therefore there should be no problems applying the DLM model to these alloys.

The ferromagnetic ground-state properties of ordered and disordered Fe-Pt alloys were calculated by several authors. The most recent investigation was carried out by Major *et al.*[13] (see also references given therein). Podgorny[14] and Hayn and Drchal[15] performed ferromagnetic fixed spin moment calculations. The stabilization of a noncollinear spin-spiral magnetic configuration in local spin-density approximation (LSDA) calculations at volumes lower than the equilibrium one has been reported for ordered Fe_3Pt by Uhl *et al.*[16] where they proposed that with increasing temperature the spin-spiral configurations become increasingly populated, which causes a decreasing equilibrium volume and thus the Invar anomaly.

This model, based on the temperature averaging over all calculated spin-spiral configurations, provides a qualitatively

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correct picture of the Invar phenomena, nevertheless, it has some technical drawbacks. First of all, the statistical averaging must be carried out over all possible excited magnetic configurations, not just over the spin spirals with fixed azimuthal angles. Next, the thermodynamical ensemble, which represents the paramagnetic state of the system, includes also states, which cannot be represented by any combination of spin-spirals. However, even if such an extended program is carried out for the paramagnetic state, the results will be comparable to the disordered local moment (DLM) approach for the case of mean-field statistical averaging for systems with well defined local atomic moments in the paramagnetic state.

The DLM approach intrinsically provides the required statistically averaged physical quantities[17,18] and can easily be applied also for random and partially ordered alloys so that the use of the DLM method seems to be a natural choice. One should also note that both approaches are only justified if saddle-point approximations for the magnetic free energy of itinerant systems can be used. This means, for example, that the intrinsic local magnetic moments exist above T_c in the sense specified in unified approaches to itinerant magnetism (see Chap. 7 in Ref. 19).

The paper is organized as follows: In the next section we describe the computational methods and details of the calculation. In the third section the main results are presented and discussed. In particular we show that the DLM approach readily predicts the weakening of the magnetovolume anomaly in the ordered alloys with respect to the disordered case. It is also shown that *ab initio* DLM calculations correctly predict a decrease of ω_{s0} as the Fe concentration decreases in ordered alloys, in the same way as it has been shown earlier for disordered fcc Fe based binary systems.[6] A general discussion of the relation of the presented approach to the overall state of art in modern Invar research is given in the last section.

II. CALCULATIONAL DETAILS

The electronic structure, total energies, and densities of states (DOS) of ordered and disordered Fe-Pt Invar alloys are calculated using the *ab initio* Korringa-Kohn-Rostoker (KKR) method in the atomic-sphere approximation (ASA) as described in more detail in Refs. 20 and 21. Effects of exchange and correlation are treated within the framework of the local spin-density approximation (LSDA) employing the parametrization by Vosko *et al.*[22] As in our previous studies[6] of disordered Fe-based Invar alloys with the TB-LMTO (tight-binding–local muffin-tin orbital) code, the radii of Fe and Pt ASA spheres are set to be equal and an *spd*-basis set is used. The coherent potential approximation (CPA) was used to treat both the effects of chemical and magnetic disorder. All calculations has been converged using a mesh of 3375 k points in the full Brillouin zone of the $L1_2$ structure which ensures an accuracy better than 10^{-3} a.u. in the equilibrium lattice constant (or the respective atomic Wigner-Seitz radius).

In order to calculate the spontaneous volume magnetostriction ω_{s0} the equilibrium volume of the paramagnetic states was determined using the disordered local moment approach (DLM).[17] The idea of the DLM formalism is to represent magnetic disorder within the CPA by treating a binary Fe_cPt_{1-c} alloys as a pseudoternary alloy $Fe_{c-x}{}^{+}Fe_x{}^{-}Pt_{1-c}$, where $c-x$ is the concentration of Fe atoms with up spin (Fe^+) and x of those with down spin (Fe^-). According to the procedure discussed earlier in more detail in Refs. 5 and 6 ω_{s0} is calculated as

$$\omega_s = \frac{V_{FM} - V_{DLM}}{V_{DLM}}, \tag{1}$$

where V_{FM} and V_{DLM} are the calculated equilibrium volumes of ferromagnetic (FM) and DLM states, respectively, where the paramagnetic DLM state is calculated for $x=1/2$.

The ordered Fe_3Pt alloy was modeled using Cu_3Au unit cell, with Pt on Au (I) sites and Fe on Cu (II) sites. For ordered alloys with higher Pt concentration the excess of Pt atoms has been equipartitionally distributed on Fe (II) sites. This corresponding to maximal possible chemical ordering. For the reason described in the introduction for the case of Fe_3Pt compositions we have also investigated partially ordered alloys of the same compositions. To do that we introduced Fe antisites in Pt position and the remaining Pt atoms were distributed on Fe (II) sites. In order to describe the degree of chemical order in the latter case the renormalized chemical long-range-order (LRO) parameter is defined in the usual way for site I as

$$S = \frac{c(\mathrm{Fe}) - c^I(\mathrm{Fe})}{c(\mathrm{Fe})}, \tag{2}$$

where c(Fe) is total concentration of Fe in the alloy and c^I (Fe) is a concentration of Fe atoms on Pt site I, thus LRO parameter S is a measure for the relative number of Fe antisites. The case of $S=0$ corresponds to the fully disordered alloy and $S=1$ to the chemically ordered one.

In our calculations the scalar relativistic approximations has been used. The values for ω_{s0} for random alloys are therefore 20–30 % larger than those which were calculated earlier[5] using the nonrelativistic TB-LMTO formalism. At the same time the calculated equilibrium lattice constants for the FM ground state is closer to those for disordered Fe-Pt by Hayn and Drchal[15] obtained from scalar relativistic TB-LMTO calculations. It should be noted, however, that it is essentially impossible to obtain an accurate description of the ground-state properties of Fe_3Pt from any approximate description of the exchange-correlation effects. On the other hand, the quantitative picture of the magnetovolume effect remains the same and is generally found to be not too sensitive to details of the calculations since only differences of volumes are involved. Besides, the experimental determination of ω_{s0} is a very subtle procedure,[1] which involves model assumptions concerning the volume of the paramagnetic state at $T=0$ K and is therefore subject of similar uncertainties as *ab initio* estimations.

III. RESULTS AND DISCUSSION

Although even in carefully prepared samples of ordered Fe_3Pt always 5–10 % of Fe atoms are at Pt sites,[23] there is

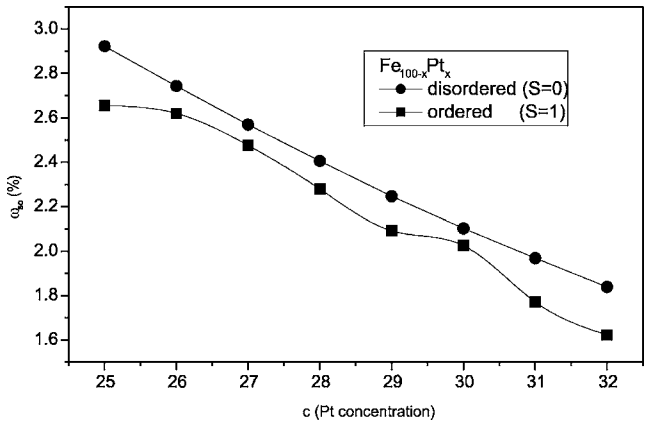

FIG. 1. Calculated ω_{s0} for ordered and disordered Fe-Pt alloys.

still a difference between disordered and ordered alloys with a high value of the chemical long-range-order parameter. This difference concerns the values of ω_{s0} and most notably of T_c as observed[4] for samples with less Fe content. In order to see how the degree of chemical order in Fe-Pt alters the value of the spontaneous magnetostriction we have performed calculations varying the long-range-order parameter S in Fe_3Pt ranging between $S=0$ (full disorder) and $S=1$ (fully ordered Cu_3Au structure). Our results show the continuous monotonic reduction of ω_{s0}. This behavior can be well explained by the differences in the DOS between ordered and disordered compositions.

The $Fe_{0.75}Pt_{0.25}$ alloy undergoes an ordering transition at about 1100 K into the $L1_2$ (Cu_3Au-type) structure. The existence region of the ordered fcc γ-Fe phase overlaps that of the disordered phase by at about 2% towards the Fe richer composition.[24] The experimentally estimated[1,2,4] spontaneous volume magnetostriction ω_{s0} has its maximum value in this small composition range and gradually decreases with growing Pt concentration both for ordered and disordered alloys. Together with a simultaneous increasing of the magnetic transition temperature this lead to a weakening of the Invar anomaly.[4] In the region of the Invar compositions ($c_{Pt}<0.32$), where both kinds of alloys can be prepared, the estimated ω_{s0} is approximately 10% larger for the disordered alloy than for the corresponding ordered one with the same atomic content.[4]

In Fig. 1 we show the calculated ω_{s0} for ordered and random Invar Fe-Pt alloys for several chemical compositions in Fe-rich region. The quantitative comparison of the values presented in Fig. 1 with experiment shows that they are 50–60 % larger. A comparison of the calculated values with available experimental estimates for ordered and disordered alloys is presented in Table I. It can be readily verified, however, that the concentration dependence of calculated ω_{s0} follows quite well the experimentally observed trends. We also obtain a difference of about 10% between ordered and disordered cases at a fixed alloy composition. It thus appears that the DLM approach provide the common description of the magnetovolume anomaly in ordered and disordered Fe-Pt alloys.

The physical mechanism of the Invar anomaly is not connected with chemical ordering in the system, although the chemical disorder is always present in real Fe_3Pt alloys, as has been discussed above. In fact it can be shown that the occurrence of the anomalous spontaneous volume magnetostriction of ordered Fe-Pt can be understood from electronic structure arguments similarly as it has been done previously for disordered alloys.[6]

TABLE I. Experimental estimations of $\omega_{s0}(\%)$ for ordered and disordered Fe-Pt from Sumiyama *et al.* (Ref. 4). The calculated values are given in brackets.

Composition	ω_{s0} disordered	ω_{s0} ordered
$Fe_{72}Pt_{28}$	1.50 (2.40)	1.34 (2.28)
$Fe_{70}Pt_{30}$	1.40 (2.10)	1.25 (2.03)
$Fe_{68}Pt_{32}$	1.25 (1.83)	1.1 (1.62)

In order to take a closer look at these issues we have calculated the dependence of ω_{s0} on the degree of chemical order in Fe_3Pt. In Fig. 2 the dependence of ω_{s0} of the long-range-order parameter is shown. It is obvious that the effect of the LRO on ω_{s0} is small: it drops only by about 10%. The only essential mechanism, relevant to the Invar anomaly, is a reduction of the local magnetic moments induced by the effects of thermal magnetic disorder.

In the ferromagnetic ground (FM) state of chemically disordered Fe_3Pt the calculated moments per atom are $M=2.08\mu_B$/atom (atomic moments on Fe and Pt are $M_{Fe}=2.68\mu_B$/Fe and $M_{Pt}=0.28\mu_B$/Pt) whereas in the corresponding DLM state the average local atomic moment

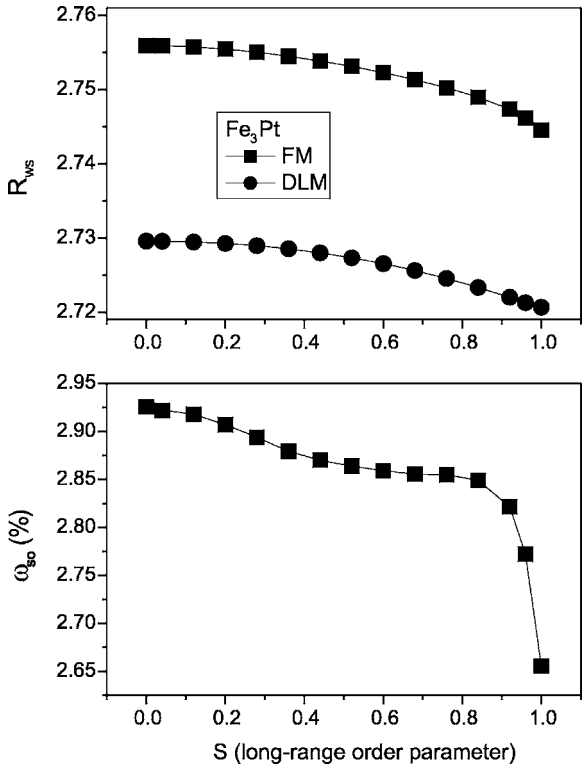

FIG. 2. Calculated dependences of equilibrium Wigner-Seitz radii (upper panel) and ω_{s0} (lower panel) on chemical long-range-order parameter in Fe_3Pt alloy.

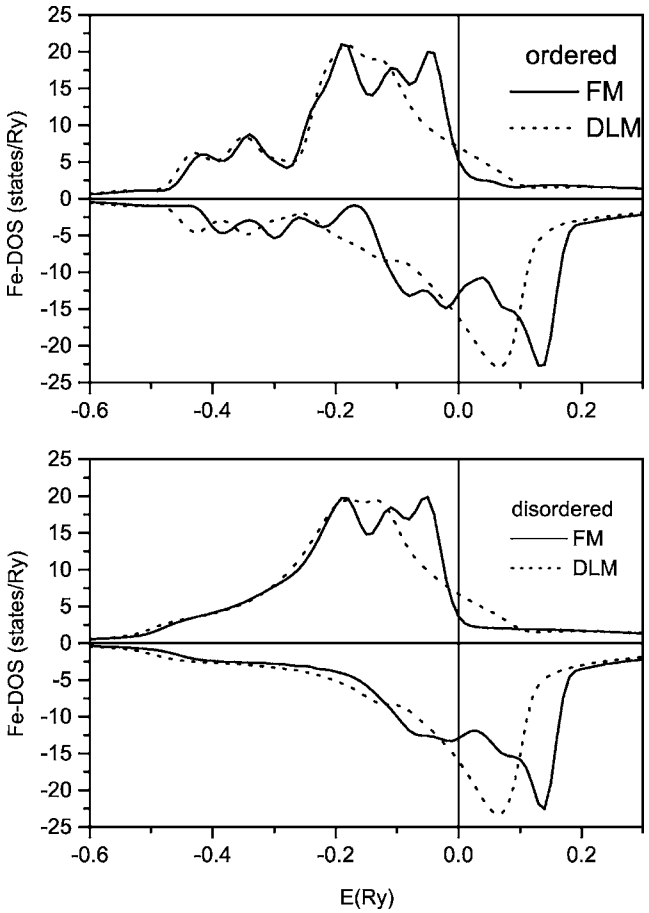

FIG. 3. Calculated DOS of FM and DLM states at their equilibrium volumes of ordered (upper panel) and disordered (lower panel) Fe_3Pt alloy.

amounts to $M=1.72\mu_B$/atom ($M_{\mathrm{Fe}}=2.30\mu_B$/Fe and zero moments on Pt sites). The magnetovolume effect connected to the reduction of the Fe local moment in the paramagnetic state as compared to the FM state (the vanishing of the induced Pt moment also contributes to the effect but at much lesser extent) causes an Invar anomaly (see also Ref. 6).

The similar but a bit smaller reduction of the moments occurs in ordered Fe_3Pt: $M(\mathrm{FM})=2.04\mu_B$/atom and $M(\mathrm{DLM})=1.70\mu_B$/atom, or $M_{\mathrm{Fe}}(\mathrm{FM})=2.62\mu_B$/Fe and $M_{\mathrm{Fe}}(\mathrm{DLM})=2.26\mu_B$/Fe. On the upper panel of the Fig. 2 the actual calculated equilibrium atomic Wigner-Seitz radius (R_{ws}) are shown. The reduction of the equilibrium R_{ws} (or equivalently of the lattice constant) by passing from disordered to ordered composition is seen for both FM and DLM states. The decrease of ω_{s0}, defined by Eq. (1) in which the FM and DLM equilibrium R_{ws} enters via the volumes is caused by a slightly stronger decrease of $R_{ws}(\mathrm{FM})$.

For ordered Fe_3Pt the anomalously high value of ω_{s0} can be understood on the same footing as for disordered alloys namely from the analysis of the local atomic DOS,[6,8] which shows that the Invar effect in ordered and disordered alloys has the same electronic origin. In Fig. 3 the local density of states (DOS) of Fe in the ferromagnetic and DLM hosts is compared for ordered (upper panel) and disordered (lower panel) Fe_3Pt. In the ordered case the reduction of the local

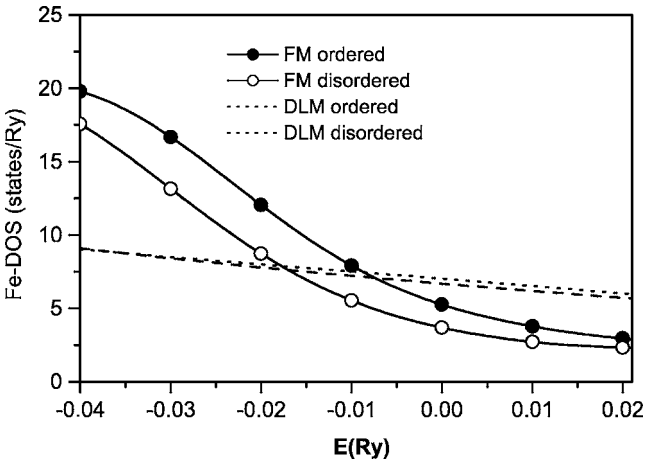

FIG. 4. Calculated majority-spin DOS of FM and DLM states of ordered and disordered Fe_3Pt in close vicinity of the Fermi level.

magnetic moment in the paramagnetic state occurs due to smoothing the DOS caused by the effects of magnetic disorder. This leads to the transition from strong ferromagnetism (the majority spin band is nearly fully occupied) for the $T=0$-K FM state to weak magnetism where part of majority band is empty. This effect in turn causes the essential reduction of the local magnetic moment on Fe in the paramagnetic state and consequently leads to a large magnetovolume anomaly.

This effect is of a similar size as in the disordered Fe_3Pt as can be seen in the lower panel of Fig. 3. The only essential condition for the appearance of the Invar anomaly is a position of the Fermi level at the top edge of the majority spin band. It is interesting to note that *ab initio* densities of states, as presented in the upper panel of Fig. 3, reproduce well the changes in the DOS between the ferromagnetically ordered state below T_c and paramagnetic state above T_c, which has been observed in angle-resolved photoemission (ARPES) experiments on ordered Fe_3Pt,[25] where significant changes in the ARPES spectra were observed upon measurements at $0.58T_c$ and $1.3T_c$. Our results also confirm the interpretation of these experiments given by Kakehashi,[26] who has questioned the original interpretation[25] given in terms of the two-state model.

The difference in the value of the magnetostriction between the chemically ordered and disordered cases comes from the fact that in the ordered composition a small portion of the majority band in the FM state is left unoccupied. In Fig. 4, where the majority spin-band DOS is shown in close vicinity of the Fermi level, this situation is illustrated even more clearly. While in the DLM state the DOS of both ordered and disordered alloys are very similar, the Fermi level of ferromagnetic DOS of disordered alloy is closer to the top edge of the majority band than in the case of the ordered alloy. It thus appears that the physical mechanism of the effect is similar in both ordered and disordered alloys—namely a reduction of the local moments induced by the thermal magnetic disorder. The DLM results provide an adequate description of this mechanism and also allow us to

understand the difference in size of the effect between ordered and disordered Fe-Pt alloys.

IV. GENERAL DISCUSSION AND CONCLUSIONS

The *ab initio* approach to the Invar related properties presented here may be regarded as a first-principle extension of the theory by Kakehashi.[27,28] The basic result of this theory is that the reduction of the volume with temperature in Invar systems is due to concomitant reduction of the local magnetic moments caused by effects of thermal disorder. The *ab initio* DLM formalism based on density-functional theory as proposed by Gyorffy *et al.*[17] very well captures this reduction of the local moment and predicts in detail a corresponding reduction of the equilibrium volume as thermal magnetic disorder increases.[5]

This model applies to the case when well defined local atomic moments occur in the system like in the fcc Fe-Pt alloys. Fe-Ni in contrast, as mentioned earlier, does not belong to this category because of the distinctive highly itinerant character of the Ni magnetism, which, in the paramagnetic regime in contrast to Fe, does not possess a local moment in the Anderson sense (see Ref. 19, Chap. 7). The attempt[29] to analyze the Invar properties using *ab initio* ground-state calculations for Fe-Ni by applying the Murata-Doniach type of spin-fluctuation theory valid for very weak itinerant ferromagnets may have only limited success since the Fe moments in Fe-Ni alloys are strongly localized.

We would like to mentioned another point of view on the Invar problem in Fe based alloys concerning the explanation of the Invar effect based on the hypothesis proposed by Weiss[30] about the existence of two separated energy minima with different volumes and magnetic states, high-spin (HS)–high-volume and low-spin (LS)–low-volume states. In this model it is assumed that thermal excitations between the HS ground-state minimum (with larger volume) and the LS state with smaller volume should lead to a negative contribution to the thermal expansion. Despite considerable difficulties which this model has from a general thermodynamical point of view (thermodynamic instability of the system, required existence of different regions with different spin state and volume[31]) the Weiss model has been revived in the late 1980s due to *ab initio* calculations of Moruzzi and co-workers[32,33] who showed that the total energy of fcc Fe and Fe-Ni Invar alloys has indeed two metastable LS and HS minima with different volumes if one constrains these systems to be ferromagnetic during the calculations.

The collinear ferromagnetic constraint imposes such two minima, which have been found also in ordered[14] and disordered[15] Fe-Pt Invar compositions. However, it has also been realized that in pure fcc Fe in a considerable volume range noncollinear antiferromagnetic states are stabilized rather than ferromagnetic ones.[34–36] The interplay between antiferromagnetic (AF) and ferromagnetic interactions in Fe-Ni Invar alloys leads to the existence of a continuum of stable noncollinear magnetic configurations as it has been shown in the calculations by van Schilfgaarde *et al.*[37]

In disordered $Fe_{72}Pt_{28}$ Invar alloy the stabilization of the effective AF interactions occurs at volumes lower than the equilibrium FM suggesting that there is no low volume LS metastable minimum.[38] It thus appears that the two-state model of the Invar anomaly has no *ab initio* justification except those provided by artificially constrained calculations. The theoretical development during the last decade has stimulated some interesting experimental investigations with classical fcc Fe based Invar alloys, which are intended to check for the proposed Invar effect scenarios. In case of the Fe-Pt system neutron-diffraction studies have been performed by Brown and co-workers,[39,40] who have shown that there are neither hidden HS-LS excitations nor any noncollinear spin configurations at elevated temperatures in Fe-Pt alloys. These experiments[40] have also shown that the population of e_g and t_{2g} orbitals stays constant with temperature in the $Fe_{72}Pt_{28}$ alloy so that no evidence of the scenario of Invar effect proposed originally by Kaspar and Salahub[41] and developed further by Entel *et al.* [42] could be found.

In this paper we have shown that the Invar anomaly can be very well understood and quantitatively described on a similar background for ordered and disordered Fe-Pt alloys. The Invar anomaly is due to reduction of the local atomic moments with temperature associated with electronic structure changes induced by the effects of thermal magnetic disorder. These changes are well captured by the DLM formalism for systems where the intrinsic local moments exists in the DLM state independently on the degree of chemical disorder. Our calculations correctly predict the weakening of the Invar anomaly in Fe-Pt for increasing chemically disorder as well as the reduction of ω_{s0} with increasing Pt concentration in both the ordered and disordered case.

Taking into the account previous successful applications of the present approach to disordered fcc Fe-Pd and bcc Fe-Co,[6] as well as previous related work on Fe-Ni alloys,[9,11] and considering also the original phenomenological treatment by Kakehashi,[27,28,43] (see for review Ref. 44) it thus appears that Invar phenomena can be understood well in the context of the general theory of itinerant magnetism[19] as being induced by fluctuations of the magnitude of the local magnetic moments with temperature.

The changes of the local magnetic moments with temperature are an intrinsic property of any magnetic system where the same electronic states simultaneously take part in the magnetic moment formation and the chemical bonding. The Invar anomaly appears when these local moment changes become anomalously large, which happens for some compositions of Fe-based alloys, due to certain combinations of electronic structure related factors as described above and elsewhere.[6]

The problem of formulating a general understanding of the Invar effect is related to the complexity of the general theory of itinerant electron magnetism itself rather than to some intrinsic peculiarities, which should exist only in Invar materials (e.g., hidden excitation), which, however, still remain experimentally unverified.

ACKNOWLEDGMENT

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