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First-principles prediction of piezomagnetic effect in the metal phase at the earth's core conditions

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Ab initio electronic structure calculations of the crystallografically ordered $FeNi_3$ at zero temperature and high pressures are performed. A magnetic collapse in $FeNi_3$ at the Earth's inner core pressure is predicted followed by the restoration of the magnetization at a higher pressure. It is shown that the enhanced filling of the narrow Fe *d* subband with compression leads to a radical reconstruction of the electronic structure and, therefore, causes these two effects.

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I. INTRODUCTION

Planetary physics deals with the problem of the chemical composition and structure of the planet's deep interior in connection with the origin and basis of the planet's magnetic field. Up to now both the chemical composition and the crystal structure of the Earth's inner core (IC) remain essentially unknown. This reason further was the primary motivation of the present study of magnetic properties of the IC. In addition, under extreme pressures some chemical elements behave differently than under ordinary conditions. Under pressure the Coulomb interaction changes, which leads to changes in bandwidths, band gaps, occupation numbers, etc., and results in interesting physical properties of the crystals. This also makes the present study interesting for materials science.

It is generally accepted that the composition of the Earth's core is similar to one of the iron-nickel alloy based meteorites, which contain, on the average, 90% Fe and 10% Ni. More than 30 years ago it was found[1] that in the pressure range from 1.5 to 3 Mbar the density of nickel is about 7% larger than the density of iron. That is not very surprising because the electronic structures of the two neighboring transition metals should not differ significantly under extreme pressures. Thus the difference in the densities should result from the difference of their atomic weights, which is about 5%. This suggests that the IC may be enriched by nickel (because that minimizes the gravitation energy), thereby making it necessary to consider also Ni-based alloys. Some geophysically important properties of the iron rich Fe-Ni alloys were studied experimentally earlier.[2]

Previously I proposed a hypothesis concerning the chemical composition and crystal structure of the IC.[3] I assumed that at least one spherical layer of the inner core may contain an iron-nickel alloy with the permalloylike chemical composition of $FeNi_3$ in an extremely compressed state. In that previous investigation I restricted myself to the calculation of the electronic structure of the compound with a density of 13 g/cm^3 corresponding to the estimated density of the IC,[4] i.e., I considered the volume compression by a factor of about 1.5. I found that this compound demonstrates a pure itinerant ferromagnetism that originates from the valence band structure only.

In the present study I focus on the theoretically predicted ferromagnetic behavior of this compound within the geophysical estimates of the IC densities on the basis of *ab initio* electronic structure calculations of the $FeNi_3$ compound. These are, to my knowledge, the first calculations reported for ferromagnetic Fe-Ni alloys under very high pressure. The magnetization obtained varies very strongly with density. I make an attempt to present a clear physical interpretation of this strange behavior.

In Ref. 3 I performed non-spin-polarized scalar-relativistic electronic structure calculations for the ground state of some crystallografically ordered stoichiometric close-packed Fe-Ni compounds with several values of the concentration of Fe. The lattice constants of all of these compounds originating from the fcc structure were chosen to provide the same mass density (13 g/cm^3). When the lattice is compressed the *d* band is expected to broaden owing to the enhanced overlap of neighboring orbitals. However, an interesting trend was revealed when the concentration of Ni is increased: the Fe *d* bands become narrower and the density of states (DOS) grows. Moreover, the compound $FeNi_3$ exhibits, first, a distinct peak in the occupied valence band in the vicinity of the Fermi level E_F and, second, a sizable Fe DOS at E_F, $N(E_F)=2.53$ states/eV atom. This situation is similar to those in non-spin-polarized calculations for Fe, Co, and Ni at ambient pressure, where $N(E_F)$ values lie in the range from 2 to 4 states/eV atom.[5]

This unusual effect can be understood in the following way. Calculations that neglect the hybridization between iron and nickel orbitals demonstrate that the lower part of the valence band, $E-E_F<-1$ eV, originates mostly from the Ni *d* states. The Fe *d* states form a narrow band (a half-width of 2 eV), which is partially occupied. Though the distance between neighboring Fe atoms in that alloy (5.847 a.u., i.e., the lattice constant) is larger than that in the bcc Fe under ambient pressure (4.680 a.u.), it should be noted that the distance between neighboring Fe and Ni atoms is only 4.135 a.u. The Fe $3d$ electrons are affected by a strong repulsive potential of the Ni sphere, and vice versa, and atomic spheres of each sort of atom is weakly transparent for the electrons of the other sort. The increase of $N(E_F)$ is directly connected to this effect.

The quantity $I(E_F)N(E_F)$, where $I(E_F)$ is the Stoner parameter, is well known to provide a direct criterion of ferromagnetic ordering, which makes it necessary to perform a spin-polarized band structure calculation of the ground state of this compound. The energy band structure for the alloy of a mass density of 13 g/cm^3 can be found in my previous paper.[3] Should the IC be made only of the $FeNi_3$ compound at zero temperature, then the theoretically predicted saturation magnetization in this compound would lead to the value of the geomagnetic field 12.3 times greater than the experimentally observed value.

The paper is organized as follows. The results on the electronic structure of the ordered $FeNi_3$ alloys at the IC conditions are presented in Sec. II. Section III discusses the predicted magnetic behavior in connection with the behavior of some magnetic compounds at ambient pressure. In Sec. IV I briefly summarize the results obtained.

II. METHOD OF CALCULATION

In the present paper I perform *ab initio* self-consistent fully relativistic spin-polarized electronic structure calculations (SpRLMTO) of the ground state of the $FeNi_3$ compound at the range of geophysically estimated mass densities of the IC. These results are important for the construction of the picture of the IC. The following assumptions are made: first, that this compound possesses a close-packed crystal structure of Cu_3Au type that originates from the fcc structure of pure Ni, and holds at ambient conditions; second, that this structure remains practically unchanged over the whole range of densities; and third, that disorder effects are negligible.

Details of the band structure calculations were the same as in my previous papers.[3,6] The angular-momentum expansion of the trial function was up to $l=2$.

Density-functional formalism produces, in principle, exact ground state properties. However, the exchange-correlation interaction is known only approximately. In the present study I use the energy functional of von Barth and Hedin[7] without relativistic corrections [the local spin density approximation (LSDA)]. It is commonly accepted that gradient corrections to the LSDA do not strongly affect the band energies and the spin magnetization, but they are important for the total energy.[8] Moreover, as pointed out in Ref. 9, at smaller volumes the charge-density gradient is, in general, smaller. In addition, I believe that the nonsphericity of the spatial distribution of the electron- and spin-magnetization densities should be small because of the enhancement of the *d* electron delocalization under the pressures considered. The spherical approximation is, therefore, plausible. These assumptions significantly simplify the computer simulation; the errors they introduce are apparently smaller than the error due to the uncertainties in chemical composition and crystal structure. I believe that these assumptions do not considerably affect the ultimate results.

I have chosen the magnetization along the [111] direction similar to the ordered $FeNi_3$ at normal conditions, where the easy axis of magnetization is [111].[10] Owing to the strong compression of the crystal lattice the Brillouin zone (BZ) volume increases and the valence band broadens. I used 1547 points in the irreducible wedge of the BZ (IBZ), which for the [111] direction of magnetization comprised 1/12th of the BZ. The self-consistency criterion was chosen to be $10^{-5}e$. That choice of parameters is necessary to ensure the convergence of the self-consistent procedure in total energy. The atomic sphere radii were chosen equal in all calculations.

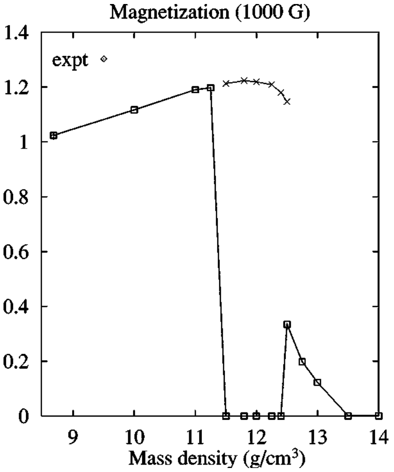

FIG. 1. Total magnetization as a function of mass density for $FeNi_3$ with the magnetization directed along [111]. Squares indicate the stable ferromagnetic solutions, and crosses correspond to the metastable ones.

III. RESULTS: ELECTRONIC AND MAGNETIC STRUCTURES OF $FeNi_3$ AT THE EARTH'S INNER CORE DENSITIES

The most interesting result is that this investigation reveals a pronounced hydrostatic pressure effect on the calculated total magnetization, see Fig. 1. Under normal conditions fcc Fe-Ni alloys with Fe concentrations lower than 45 at % are collinear ferromagnets.[11] First, it should be noted that the agreement between the calculated and experimental values for the ambient conditions is excellent.[12] Second, the weak growth of the magnetization in the range from ambient pressure (8.68 g/cm^3) up to 11.25 g/cm^3 is explained simply by the fact that with increasing pressure the magnetic moments on iron and nickel sites decrease more slowly than the unit cell volume does. Note that this fact corresponds to the experimentally observed positive value of the pressure derivative of the Curie temperature.[12] On the other hand, the theoretically predicted magnetization of the random $FeNi_3$ alloy under normal conditions is only 4% less than for the ordered one.[13] So it is quite possible that experiments on $FeNi_3$ will show a weaker increase of the magnetization with pressure at about 10 g/cm^3 than was obtained in my collinear spin-polarized calculations for the ordered alloy. This may be due to the chemical disorder at relatively low pressures, as described in Ref. 13.

Much more surprising is the presence of a pronounced gap in a range from 11.3 to 12.4 g/cm^3. This means that the ferromagnetic ordering in the ground state disappears abruptly at around $\rho=11.3$ g/cm^3, and that spin alignment is restored at around $\rho=12.4$ g/cm^3 (Ref. 6). Still more surprising is the sharp increase of the magnetization as the density increases from this value. Thus we observe a recovery of the ferromagnetic behavior. As the density further increases (and the volume decreases) the magnetization decreases, the

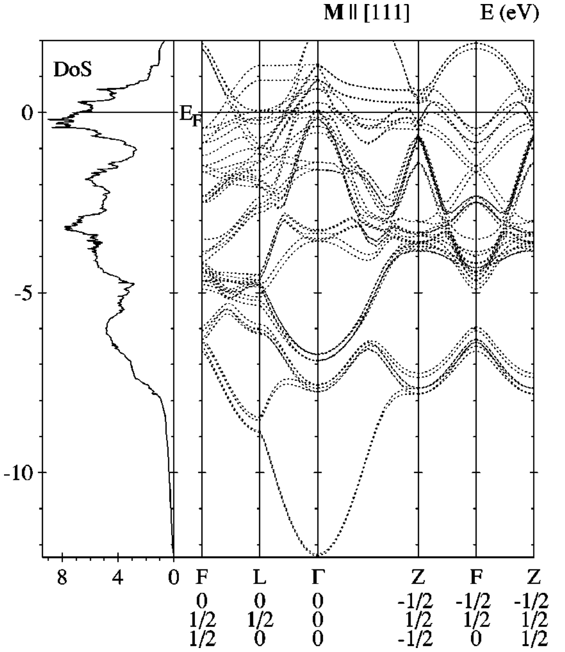

FIG. 2. $FeNi_3$ low spin energy bands for the mass density equal to 12.5 g/cm^3 with the magnetization along [111] and the total DOS (in units of states/eV).

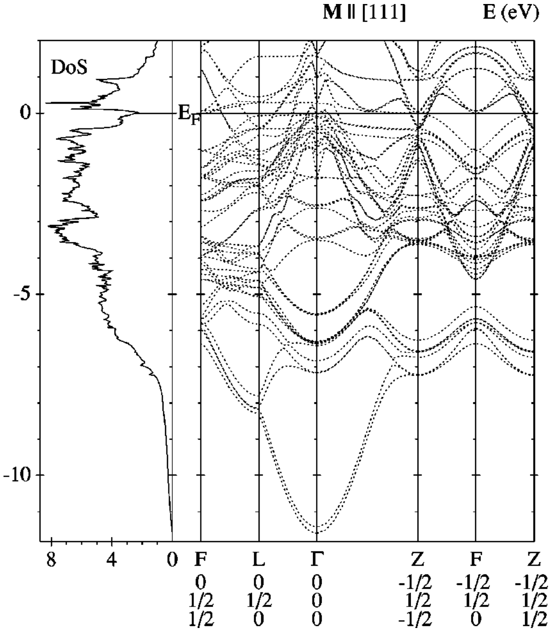

FIG. 4. $FeNi_3$ high spin energy bands for a mass density equal to 11.25 g/cm^3 with the magnetization along [111] and the total DOS (in units of states/eV).

dependence being nonlinear. Thus the magnetization reaches a maximum value at a density near 12.5 g/cm^3 which is about three times smaller than the magnetization at ambient pressure. The actual value may be larger: it is well known that the currently used LSDA, in general, underestimates magnetic stabilization energies in comparison with the generalized gradient approximation. The sharp decrease followed by the recovery of the magnetization are in strong contrast to the lowering of the magnetization of $3d$ ferromagnetic metals (and Fe-Ni alloys) with compression above the ambient pressure. We can conclude that a series of pressure induced quantum phase transitions takes place at zero temperature.[14]

We infer that here we encounter a piezomagnetic effect in the itinerant ferromagnet. Note that up to now a piezomagnetic effect was experimentally observed only in antiferromagnets. In this connection note that usually an origin of the ordinary piezomagnetic effect lies in anisotropic forces arising from crystallografically inequivalent sites. Contrary to this, here we see the effect at *hydrostatic* compression, due to an oscillatory dependence of the exchange-correlation interaction, as will be discussed further below. Hereafter we make

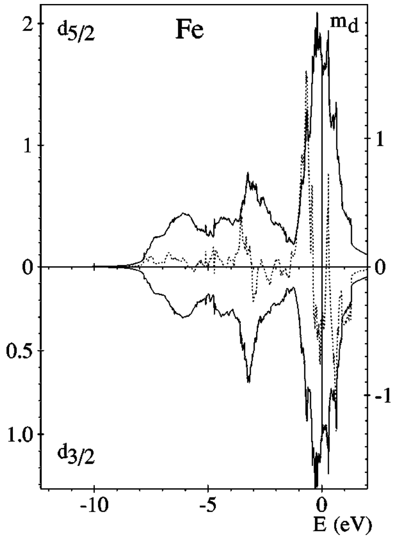

FIG. 3. d partial densities of states (solid curves, scale at the left in units of states/eV atom) and d partial densities of the spin magnetization (dashed curves, scale at the right in units of μ_B/eV atom) for a mass density equal to 12.5 g/cm^3.

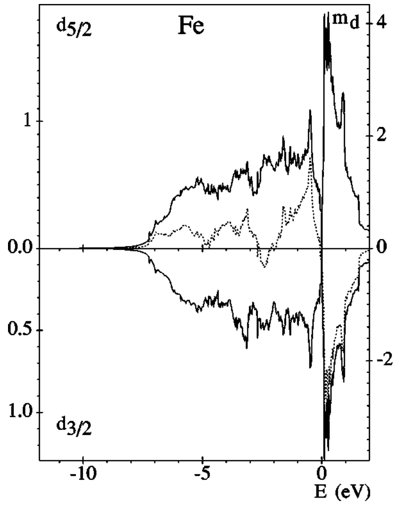

FIG. 5. d partial densities of states (solid curves, scale at the left in units of states/eV atom) and d partial densities of the spin magnetization (dashed curves, scale at the right in units of μ_B/eV atom) for a mass density equal to 11.25 g/cm^3.

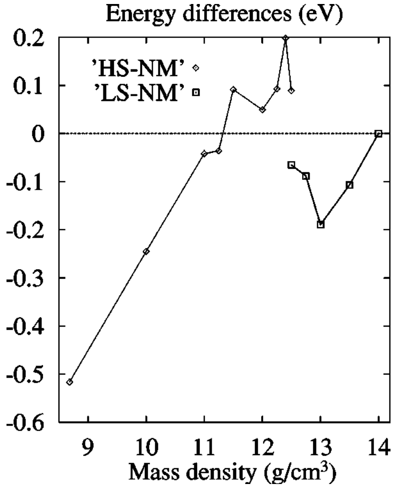

FIG. 6. Calculated total energy differences between the HS and NM states for Cu_3Au crystal structure of $FeNi_3$ as a function of mass density.

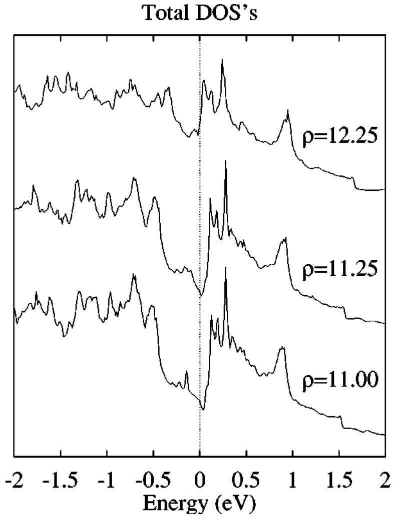

FIG. 7. Blowup of the total DOSs of ferromagnetic $FeNi_3$ near the Fermi level for three values of the mass density corresponding to stable ($\rho = 11$, and 11.25 g/cm^3) and metastable ($\rho = 12.25$ g/cm^3) solutions.

an attempt to rationalize the effect.

Figure 2 represents the energy bands along the high-symmetry directions and the total DOS at the lattice parameter of 5.924 a.u. corresponding to a mass density equal to 12.5 g/cm^3 and possessing the largest magnetization of 1.113 μ_B/cell in the high density range. The partial DOSs and the energy dependence of the spin magnetization are shown in Fig. 3. Although the energy band structure is very similar to those for the density of 13 g/cm^3 (Ref. 3), the total magnetization is about 2.7 times larger than for that density.

This is a scenario we can see in Fig. 1. Strictly speaking, as the density increases from its value at ambient pressure, the ferromagnetic solution never disappears completely up to 13.5 g/cm^3. That is, high spin (HS) ferromagnetic solutions (see Figs. 4 and 5) exist not only in the range from ambient pressure (8.68 g/cm^3) up to 11.25 g/cm^3 (which are denoted by squares) but also in the range from 11.25 up to 12.4 g/cm^3 (crosses). However, Fig. 6 shows the calculated differences of total energies (per formula unit) of magnetic and nonmagnetic (NM) solutions on the density. We can see that in this range from 11.3 up to 12.4 g/cm^3 the total energies of the HS states exceed those of the NM states, which are more energetically favorable here. As an example, the corresponding local Fe and Ni DOSs of the NM solution can be found in Ref. 3.

An origin of this magnetovolume effect may be understood in the following way. The enhanced filling of the narrow Fe *d* subband with compression (see Fig. 5), due to the small charge transfer from Ni to Fe atoms plays a decisive role in the magnetic behavior of $FeNi_3$ in this region. Figure 7 represents the mass density dependence of the total DOSs of the ferromagnetic $FeNi_3$ in the vicinity of the Fermi level. Evidently, the smaller the unit cell volume the larger the Fermi energy. However, when the mass density increases up to 11.25 g/cm^3, E_F still falls into a narrow valley of the total DOS, originating from the narrow Fe *d* partial DOS, and we observe a HS ferromagnet. As the mass density increases further, E_F starts to fall onto the low energy slope of the large peak of the DOS (mainly Fe *d* states), as we can see in Fig. 5 for $\rho = 12.25$ g/cm^3. Certainly this leads to an enhancement of the band energy of the valence electrons $\int^{E_F} EN(E)dE$ and, accordingly, of the total energy of the solid, which cannot be compensated by a decrease of the exchange-correlation (magnetic) energy.[15] This makes the spin alignment energetically unfavorable and the ferromagnetic solution disappears, which explains the nature of the pressure induced collapse of the magnetization upon reaching a density of 11.3 g/cm^3. In this context the energy difference should be considered only as an estimate, as the actual magnetic state at this range seems to be a disordered local moment state, as will be discussed further below. Nevertheless, we may conclude that at around 11.3 g/cm^3 a strong first-order transition occurs from the HS state to some paramagnetic state.

At higher densities, when E_F passes the peak and lies on its high-energy slope (see Fig. 3), the situation radically changes. Starting at 12.5 g/cm^3 a low-spin (LS) ferromagnetic state becomes favorable (the reverse first-order transition). Hence the cusp behavior of the magnetization of $FeNi_3$ in the range from 12.5 to 13.5 g/cm^3 is intimately connected to the occupation of the *d* subband, which gradually grows with increasing pressure.

The scenario considered is somewhat similar to that in the Invar alloys of about Fe_3Ni composition. If we cut off and extract the range from 11.3 up to 12.5 g/cm^3 from Fig. 1, the picture obtained will remind us that of the magnetovolume instability observed in fcc Fe and Fe_3Ni (Ref. 16), where the transition from HS to LS states occurs discontiniously with increasing pressure.

IV. DISCUSSION

First of all, note that the compound considered possesses a Cu_3Au crystal structure originating from the fcc and consists of similar atoms. Heine and Samson showed[17] that a critical Stoner parameter for ferromagnetism I (more exactly I/W, where W is a bandwidth) has a strong oscillatory dependence on the band filling near the end of the phase diagram. Furthermore, at the end of transition metal series one observes a competition between the Stoner criterion of ferromagnetism and that of the disordered local moment state, moreover, antiferromagnetic ordering is even less probable here.

We can shed light on this highly unusual magnetic behavior from another point of view. It is generally accepted that in metallic magnets the exchange-correlation interaction is of Ruderman-Kittel-Kasuya-Yosida (RKKY) type. All HS (stable and metastable) solutions from 8.68 up to 12.5 g/cm^3 represent a strong ferromagnet with the fully occupied majority spin band (see Fig. 5), and, therefore, the exchange-correlation interaction exponentially dampens with the distance.[18] In the intermediate compression states from 11.25 to 12.5 g/cm^3 the Fermi surface is sufficiently large resulting in (i) a small (of the order of $2\pi/k_F$) period of oscillations and (ii) fast decay of the amplitude with the interatomic distance R, therefore the interaction is fairly short ranged. Both of these features should lead to spin glass behavior of the local Fe moments. Starting with 12.5 g/cm^3 the lowest energy solutions describe the weak ferromagnets (see Fig. 3) with ordinary R^{-3} decay only, existing up to 13.5 g/cm^3. It is the superposition of such kinds of RKKY interaction that yields a quasioscillatory dependence of the magnetization plotted in Fig. 1.

It is well known that under very high pressure (about 10 Mbar) the electronic structures of the majority of elements become similar due to the free-electron-like behavior of valence electrons.[3] However, under the IC core pressures about 3 Mbar we observe this effect only partly. That is, the valence electrons behavior of a certain compressed metal resembles that of another metal under atmospheric pressure.

Indeed, calculated nonmagnetic DOSs of TP_3 compounds with $T=3d$ metal and $P=$Pd or Pt in Cu$_3$Au crystal structure at atmospheric pressure[19,20] are similar to that of FeNi$_3$ (see Figs. 2 and 3). First, the valence bands have three major peaks typical for fcc metals with nearly filled bands. Second, there is a pronounced gap near 1 eV below E_F originating from a "pseudogap." Third, the Fermi energy is at a large DOS peak containing mostly the d states of the T atom.

It is worth noting that spin-polarized electronic structure calculations predict a ferromagnetic ordering in these compounds, which is mainly confirmed experimentally. The dependence of the local magnetic moments in the "magnetic" T atom on the number of its valence electrons has a clearly defined bell-like form[19,20] with a small (or zero) value of magnetization both at the beginning ($T=$Ti, V) and at the end ($T=$Ni, Cu) of the series. In the middle of the series ($T=$Cr, Mn, Fe, and Cu) the moments reach considerable values [$\sim(2.5$–$4)\mu_B$]. As shown in Ref. 19 the effect is explained by the successive filling of the T site d subband in the vicinity of E_F without a noticeable reconstruction of the electronic structure.

The filling of the narrow Fe d subband plays a decisive role also in the magnetic behavior of FeNi$_3$, the same way as in TP_3 compounds, the only difference being that in this case the number of valence electrons of the $3d$ element changes discretely with the atomic number of the T constituent. At 11.3 g/cm^3 the magnetization sharply falls to zero, which reminds of the TiPt$_3$ compound, where only a small decrease of the lattice constant destroys the spin polarization.[20]

At the same time, the compounds VPt$_3$ and CrPt$_3$, which have similar electronic structures,[20,21] demonstrate a ferrimagnetism with a small ($\sim 0.3\mu_B$) magnetic moment on the Pt atoms antiparallel to a great magnetic moment on the T atoms. To elucidate this possibility in FeNi$_3$, I have performed calculations with that spin geometry, but failed to find a ferrimagnetic solution in the pressure range considered. On the other hand, FePt$_3$ demonstrates simple antiferromagnetic alignment in corner Fe sites.[20] I have not studied such a possibility in the range from 11.3 to 12.4 g/cm^3, where the magnetization is zero, because even if the antiferromagnetic solution existed, this would not change the final conclusion about the piezomagnetic effect.

As a result of discussion above I may propose the following analysis that leads to a qualitative understanding of magnetic behavior of crystallografically ordered FeNi$_3$ compound under compression. In the range from 8.68 to 11.3 g/cm^3 the d bands of both constituent atoms broaden with increasing occupation and, therefore, the magnetic moments decrease. In this case the effect is more pronounced on the Ni atoms. At the mass density of 11.3 g/cm^3 the local moment on the Ni atom vanishes, while the local moment on the Fe atom remains finite due to the exchange-correlation interaction on the Fe atom and its sharp partial d DOS. Here one can expect a spin glass behavior of Fe moments which exists up to 12.4 g/cm^3. However, in this range of densities my theoretical predictions are less reliable, because I cannot computationally resolve all possible magnetic structures. As the density further increases, owing to the growing "compression" of the Ni atoms, the decreasing local moment of the Fe atoms remains strong enough to cause the spin polarization of the Ni valence orbitals leading to a weak (and in above sense itinerant) ferromagnetism. A further increase of pressure leads to a broadening of the Fe d subband in the vicinity of the Fermi level, and the magnetization reduces to zero at 13.5 g/cm^3 due to the zero local magnetic moment on the Fe atom. At higher densities there are zero local moments on both constituent atoms, which is a true nonmagnetic state. To conclude I think the above transitions would not be so sharp but rather more gradual.

In addition, it is obvious that the effect of pressure on the magnetization can depend on even small changes of the chemical composition of the iron-nickel host. That is, alloying FeNi$_3$ with light element impurities can move the LS magnetization peak towards either high or low mass densities. Furthermore, an effect of the impurities can tune the distinct peaks of the DOS onto the Fermi level, so that to amplify the magnetization by stabilizing the HS ferromagnetism. This is just what was observed from electronic structure calculations[22] of the close packed Fe$_3$S under the Earth's core pressures, which additionally reveal a distinct peak in the total DOS near E_F. Simultaneously, light impurities reduce the density of the alloy and, therefore, its rigidity increases.

I close this section by making a comparison between the predicted magnetic behavior of $FeNi_3$ under the Earth's core pressures with that in Invar alloys. Up to the present attention has mainly been paid to the Fe-Ni alloys close to the Invar composition (about 35-at % Ni) due to the unique physical properties at atmospheric pressure. Here, the effect of Ni is to stabilize the fcc structure of the Fe-host matrix starting with 20-at % Ni.

Most work (see, e.g., Refs. 13 and 23, and references therein) dealt with the problem of magnetism in Fe-Ni alloys within two limitations: (i) the fcc Fe-rich side of the Fe-Ni phase diagram, and (ii) the atmospheric pressure or relative small compression (about 100 kbar, where the local magnetic moment originates from the intra-atomic exchange in the free atom). Variations in the nearest neighborhood of each sort of atom and interatomic distance change the sign and the value of the inter-atomic exchange that lead to the various types of collinear, noncollinear, or spin-glass arrangement of the local moments.

The main difference between the aim of Invar investigations and that of the present paper is as follows. The former is directed to describing the distribution of the amplitude and orientation for the Fe and Ni local moments under atmospheric pressure and relatively low ones, when, as it has been stated above, these moments come from intra-atomic free atom exchange. Contrary to this, I make an attempt to explain the transition from the ferromagnet at ambient pressure through (some kind of) a paramagnetic state to the state of the weak pure itinerant band magnetism. In this connection I should note that in my consideration of pure itinerant magnetism the term ''local moment'' means an integrated spin density over an atomic sphere without any connection to the free atom magnetic moment. Thus the mechanisms of the pressure dependence of the magnetization in Invar alloys and extremely compressed $FeNi_3$ are quite different.

Now we consider the possibility of the existence of a disordered local moment state in $FeNi_3$ at low pressure similar to that found in random Fe_2Ni alloys.[23] The latter phenomenon is explained by the chemical disorder existing in these alloys. Generally speaking, this idea is well established. Let us recall the famous Bethe-Slater plot that schematically describes the value and sign of the exchange integral versus interatomic distances in $3d$ metals. Furthermore, the dependence of the exchange integral on the angular part of the wave functions was shown to be of similar importance.[24] In addition, similar conclusions were achieved in the case of noncollinear alignment and/or a disordered local moment state which was shown to be very sensitive both to atomic distance and to the lattice symmetry (e.g., Ref. 25). Accordingly, as pointed out in Ref. 26, neither the Heisenberg model of localized spins nor the Stoner theory of band magnetism can describe the Invar effect because spin fluctuations are important.

As mentioned above there is no doubt that under the Earth's core pressure a metal must possess a close packed crystal structure, very probably of Cu_3Au type originating from the fcc Ni at atmospheric pressure. If there was a phase separation of $FeNi_3$ at very high pressures into Fe- and Ni-rich phases, there would be some grounds for considering my theoretical predictions less reliable. But Cu_3Au is a very simple, close packed structure, so it is doubtful that such a phase separation really occurs. Therefore an incorrect prediction of the ground state of the $FeNi_3$ alloy does not seem probable. Chemical disorder should be also suppressed (at least at low temperatures), because in general for the close packed structures it leads to some increase of the volume. Concerning the problem of the ferromagnetic ground state note that, for example, chemically disordered fcc alloy Ni_3Mn is paramagnetic, although the ordered one (with the structure of Cu_3Au) is ferromagnetic.

Experimental verification of the above theoretical predictions would require measurements of magnetic properties at megabar pressures. The technique recently proposed in Ref. 27 seems to be appropriate for such a task. Realization of appropriate experiments would be highly desirable.

V. CONCLUSION

Based on the first-principles theory an attempt was made to predict an unusual effect resulting from the pressure induced changes in the electronic structure of a $FeNi_3$ compound under extreme pressures. That is, in *the metal phase*, with the growth of density, there are two critical points such that the spontaneous magnetization appears at the lower critical point and then disappears at the higher critical point. This is more interesting in that, according to modern planetary physics, the Earth's neighbor planets have similar cores, their core densities being smaller and their magnetic fields being considerably weaker.

The present first-principles theory predicts that ferromagnetism in the metal phase at high pressures can exist. Even the magnetohydrodynamic model of the geomagnetic field generation requires a permanent magnet to be present to start with.

It is desirable to test the theoretical predictions of the present work by developing magnetic techniques to study phenomena at megabar pressures which would shed light on the single-solid-phase model.

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