ELASTIC AND THERMAL PROPERTIES OF $FeNi_3$ ALLOY UNDER EARTH'S INNER CORE CONDITIONS

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The *ab initio* calculations of the electronic structure of crystallographically ordered alloy $FeNi_3$ at extreme pressures and various temperatures are performed. The elastic and thermal parameters of the compound are studied with the aim to compare the calculated values of sound wave velocities with the observed values of velocities of seismic waves propagating through the Earth's inner core. An attempt is made to estimate the melting temperature of the alloy.

1. 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. A. Einstein believed that the elucidation of the basis of the Earth's magnetic field is one of five most important unsolved problems in geophysics [1]. Up to now, both the chemical composition and the crystal structure of the Earth's inner core remain essentially unknown. This reason further was the primary motivation of the present study of the properties of the inner core. In addition, some chemical elements behave differently at extreme pressures than under ordinary conditions. At pressure, the Coulomb interaction changes, which leads to changes in bandwidths, band gaps, occupation numbers, etc., and results in the interesting physical properties of 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 [2] that the density of nickel is about 7% larger than that of iron in the pressure range from 1.5 to 3 Mbar. That is not very surprising because the electronic structures of the two neighboring transition metals should not differ significantly at 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 inner core 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 iron rich Fe-Ni alloys were studied experimentally earlier [3].

Previously, we proposed a hypothesis concerning the chemical composition and crystal structure of the inner core [4]. We assumed that at least one spherical layer of the inner core may contain an iron-nickel alloy with the permalloy-like chemical composition of $FeNi_3$ in an extremely compressed state. In that previous investigation, we restricted ourself 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 inner core [5], i.e., we considered the volume compression by a factor of about 1.5. We found that this compound demonstrates a pure itinerant ferromagnetism that originates from the valence band structure only. Moreover, the first-principles theory predicts a piezomagnetic effect in this ordered alloy at extreme pressures [6]. That is, there are two critical points with the growth of density 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.

In the present study we focus on the theoretical estimate of some elastic and thermal characteristics of this compound at the inner core pressures that are of interest to geophysics. In particular, we predict quantitatively the behavior of the sound velocities in $FeNi_3$ at finite temperatures and try to estimate its melting temperature. These are, to our knowledge, the first calculations reported for ferromagnetic Fe-Ni alloys at very high pressures.

The paper is organized as follows. The method of calculation of the electronic structure of ordered $FeNi_3$ alloys under the inner core conditions are presented in Section 2. Section 3 is devoted to its elastic and thermodynamics properties. The results are compared with previous calculations and with available experimental data. Finally, we present our conclusions.

2. Method of Calculation

In the present paper, we perform *ab initio* self-consistent fully relativistic spin-polarized electronic structure calculations (SpRLMTO) of the ground state of $FeNi_3$ in the range of geophysically estimated mass densities of the inner core. These results are important for the construction of a picture of the inner core. The following assumptions are made: first, this compound possesses a close-packed crystal structure of the Cu_3Au type that originates from the fcc structure of pure Ni and holds under ambient conditions; secondly, this structure remains practically unchanged over the whole range of densities; and thirdly, disorder effects are negligible. Details of the band structure calculations were the same as in our previous papers [4, 6]. The angular-momentum expansion of the trial function was up to $l = 2$. The density-functional formalism produces, in principle, exact ground state properties. However, the exchange-correlation interaction is known only approximately. In the present study, we use the energy functional from [7] without relativistic corrections [the local spin density approximation (LSDA)]. It is commonly accepted that gradient corrections to 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 [10], at smaller volumes, the charge-density gradient is, in general, smaller. In addition, we believe that the nonsphericity of the spatial distributions of the electron- and spin-magnetization densities should be small because of the enhancement of the d electron delocalization at 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. We believe that these assumptions do not considerably affect the ultimate results. We have chosen the magnetization along the [111] direction similar to the ordered $FeNi_3$ under normal conditions, where the easy axis of magnetization is [111] [9]. Owing to the strong compression of the crystal lattice, the Brillouin zone (BZ) volume increases and the valence band broadens. We used 1547 points in the irreducible wedge of the BZ, which comprises 1/12th of the BZ for the [111] direction of magnetization. The self-consistency criterion was chosen to be $10^{-4}e$. That choice of parameters is necessary to ensure the convergence of the self-consistent procedure in total energy. The atomic sphere radii of Fe and Ni were chosen equal in every calculation.

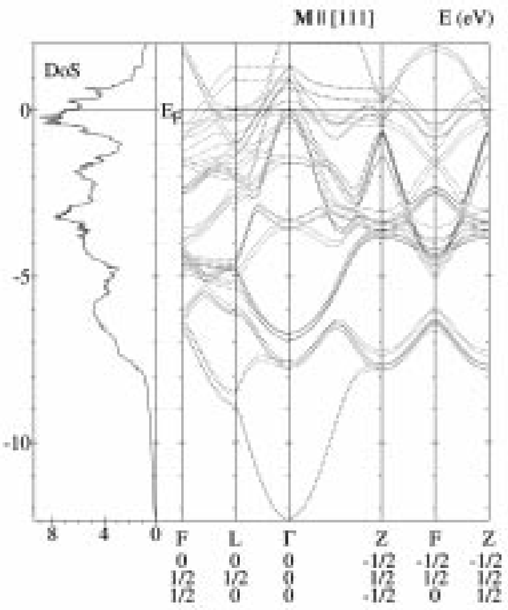

Fig. 1. $FeNi_3$ energy bands for the mass density equal to 12.5 g/cm^3 with the magnetization along [111] and the total DOS (in units of states/eV)

Fig. 1 represents the energy bands along the high-symmetry directions and the total density of states (DOS) at the lattice parameter of 5.924 a.u. corresponding to the 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. Although the energy band structure is very similar to that for the density of 13 g/cm^3 [4], the total magnetization is about 2.7 times larger.

3. Elastic and Thermal Properties of $FeNi_3$ under the Earth's Inner Core Conditions

The elastic and thermal properties of the inner core are of fundamental interest because they provide basic constraints on its structure, composition, and temperature. The temperature is intimately connected to the Earth's heat flow and to the melting process on the inner core boundary. Of particular interest is a quantitative prediction of the velocities of sound waves traveling through the core at finite temperatures because they are the only characteristics of the inner core that can be directly measured. Considering these properties of $FeNi_3$ under the inner core conditions, we start with the assumption that both inelastic effects and partial melting are absent. Secondly, we suppose that the extremely compressed metal strictly obeys the equations of elasticity theory.

It was pointed out in [11] that there is a significant difference between bulk and shear moduli. The former originates mostly from the kinetic energy of valence electrons, which is the most important contribution to the total energy. The shear moduli are determined mainly by the Coulomb interaction between ion cores; consequently, the shear to bulk moduli ratio scales as $\Omega^{1/3}$, Ω being the unit cell volume. So, metals at extreme pressures should possess small shear moduli. That is exactly the same situation that is observed for seismic shear (s) and longitudinal (p) wave velocities [5] and leads to the Poisson ratio σ slightly smaller than 0.5. Furthermore, based on the second-order elasticity theory for extreme pressures, the same conclusion was made in [12].

The differences of total energies involved in shear deformations are much smaller than those due to compression, which causes difficulties for *ab initio* methods. Even for hcp and fcc crystals of pure Fe at extreme pressures, the shear moduli from first-principles computations are reproduced only approximately [8]. Secondly, shear moduli are strongly anisotropic [11]. Thirdly, we are unable to treat the temperature dependence of the Poisson ratio, the more so that the geotherm – the temperature distribution within the inner core – is known only approximately. These difficulties can be circumvented by using the Poisson ratio derived from seismic observations at the actual temperature of the inner core (which is not known exactly), that is [13]

$$\sigma = \frac{1}{2}\frac{(v_p/v_s)^2 - 2}{(v_p/v_s)^2 - 1}, \tag{1}$$

where $v_p = 11.262$ km/s and $v_s = 3.668$ km/s according to PREM (Preliminary Reference Earth Model) [5]. The corresponding value of the Poisson ratio at the center of the inner core is 0.4407.

By employing the only phenomenological parameter σ, one can easily obtain the following expression for the longitudinal sound velocity

$$v_p = \sqrt{\frac{B}{\rho}\frac{3(1-\sigma)}{1+\sigma}}, \tag{2}$$

where B is the bulk modulus and ρ is the density.

Before the determination of the velocities from a completely *ab initio* approach, it makes sense to try to estimate their values. We use the Debye theory of harmonic lattices to estimate the temperature dependence of the physical characteristics of the inner core such as the pressure, bulk modulus, and longitudinal velocity v_p. Our starting points are as follows. First, we believe, as mentioned above, that the covalent constituent of the chemical bond of $3d$ states in extremely compressed Fe-Ni alloys is negligible; in other words, the nonsphericity of the spatial distribution of the electron- and spin-magnetization densities is small because d electrons are strongly delocalized at such pressures. This justifies the use of the Debye approach which is based on the assumption that the medium is isotropic. Secondly, under these conditions, the electron gas acquires features of an ideal gas [4], so the situation becomes somewhat similar to that in alkaline metals. Obviously, the investigation of elastic and thermodynamic properties of solids from the first principles in the vicinity of magnetovolume instabilities is very complicated problem which cannot be solved accurately at present time. However, the magnetization is small enough [6] to allow us to use the Debye theory. Thus, we expect the present approach to yield plausible results.

To proceed, we need an explicit expression for the Helmholtz free energy which looks in the standard notations as [14]

$$F(s,T) = E_r(s) + \nu k_{\mathrm{B}} T \left\{ 3\ln\left[1 - \exp\left(-\frac{\Theta_{\mathrm{D}}}{T}\right)\right] - \right.$$
$$\left. - D\left(\frac{\Theta_{\mathrm{D}}}{T}\right)\right\} + \nu \cdot \frac{9}{8} k_{\mathrm{B}}\Theta_{\mathrm{D}} - T S_{\mathrm{el}}(s,T), \tag{3}$$

where k_{B} is the Boltzmann's constant, Θ_{D} is the Debye temperature, $D(\Theta_{\mathrm{D}}/T)$ is the Debye function, ν is the number of atoms per unit cell, and s is a mean atomic radius. Here, S_{el} is the electronic entropy which has the form

$$S_{\mathrm{el}}(T) = -k_{\mathrm{B}} \int N(E)\left\{f(T,\zeta,E)\ln f(T,\zeta,E) + \right.$$
$$\left. + [1 - f(T,\zeta,E)]\ln[1 - f(T,\zeta,E)]\right\} dE, \tag{4}$$

for the ideal electron gas, where $N(E)$ is the DOS function, $f(T,\zeta,E)$ is the Fermi function at a temperature T, and ζ is the chemical potential. In Eq. (3) $E_r(s)$ is the total energy of the rigid lattice and $\frac{9}{8}k_{\mathrm{B}}\Theta_{\mathrm{D}}$ is the Debye estimate of the zero-point lattice energy. The Debye cutoff frequency is related to the Debye temperature as [14]

$$\omega_{\mathrm{D}} = \frac{k_{\mathrm{B}}}{\hbar}\Theta_{\mathrm{D}} = \bar{v}\left(\frac{6\pi^2 N\nu}{V}\right)^{\frac{1}{3}}, \tag{5}$$

where $\bar{v}$ is the average for the sound velocity (transversal and longitudinal), N is the total number of particles, and V is the system volume. In the limit that the temperature is much lower than the binding energy, the $\bar{v}$ is found from

$$\frac{3}{\bar{v}^3} = \frac{2}{v_s^3} + \frac{1}{v_p^3}. \tag{6}$$

Let us take into account the expressions of v_s and v_p in terms of shear S and bulk B moduli [13]

$$v_p = \sqrt{\frac{B}{\rho}\left(1 + \frac{4}{3}\frac{S}{B}\right)}, v_s = \sqrt{\frac{S}{\rho}} \tag{7}$$

and the relation [13]

$$\frac{S}{B} = \frac{3}{2}\frac{1-2\sigma}{1+\sigma}, \tag{8}$$

where the isothermal bulk modulus B is defined as

$$B = -V\left(\frac{\partial P}{\partial V}\right)_T, \tag{9}$$

and P is the hydrostatic pressure

$$P = -\left(\frac{\partial F}{\partial V}\right)_T. \tag{10}$$

Practical computations of the partial derivatives are made by the least-squares fit of the calculated values of the free energy to the Morse function [16]

$$F(s) = a + b\mathrm{e}^{-\lambda s} + c\mathrm{e}^{-2\lambda s}, \tag{11}$$

where a, b, c, and λ are the fitting parameters and s is the mean atomic radius. The accuracy needed to determine the bulk modulus is achieved by the fit with an rms error of at most 0.5 mRy.

Thus, ω_{D} takes the form [15]

$$\omega_{\mathrm{D}}(s) = 2^{2/3}3\pi^{5/6}\left[\frac{(1-\sigma)(1-2\sigma)}{1+\sigma}\right]^{1/2} \times$$
$$\times \frac{1}{[2^{5/2}(1-\sigma)^{3/2} + (1-2\sigma)^{3/2}]^{1/3}}\sqrt{\frac{\nu B s}{\sum_i^{\nu} M_i}}, \tag{12}$$

where M_i is the atomic mass of a component in the unit cell.

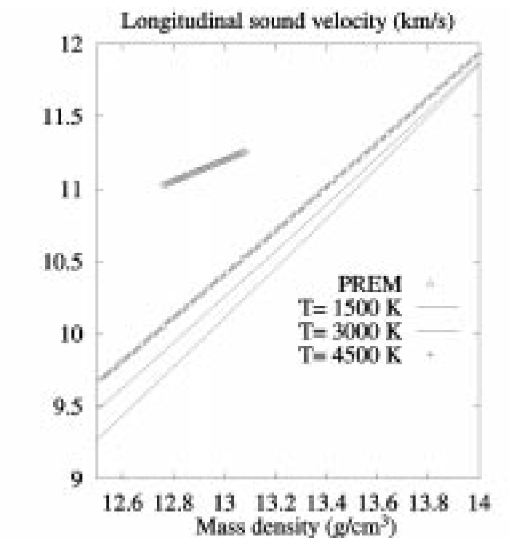

Fig. 2. Calculated longitudinal sound velocity of the ferromagnetic FeNi$_3$ along three isotherms compared with that of the inner core (according to PREM)

In many respects, our approach is similar to that used in [16]. However, there is one significant difference, namely that we use the values derived exactly from elasticity theory, in contrast to those in [16] based on the fit to the experimental data for a number of cubic metals.

With the above assumptions, $\omega_{\mathrm{D}}(s)$ [Eq. (12) together with Eqs. (3), (9), and (10] obeys a complicated second-order differential equation. We assume that for low and moderate values of the ratio $k_{\mathrm{B}}T/\hbar\omega_{\mathrm{D}}$ the physically acceptable self-consistent solution of Eq. (12) for ω_{D} is a slowly varying function of the temperature T. One should carefully identify possible solutions to this set of equations which correspond to the temperatures lower than the (unknown) melting point of the compound in question.

Fig. 2 shows the calculated dependences of the longitudinal sound velocity on the density of the inner core. As expected, our approach underestimates the velocity with respect to PREM [5]. At the density of 13 g/cm^3, the discrepancy is about 7% for T =4500 K. If we assume that the inner core is composed of pure iron in a close packed phase, the discrepancy from PREM would be about 1.6% [17], which is considerably smaller. However, the electronic structure of FeNi$_3$ at extreme pressures is quite different from that of pure Fe both in scalar-relativistic and spin-polarized calculations. Pure Fe has slowly varying DOS in the vicinity of the Fermi level (E_{F}) with the DOS(E_{F}) being about 1 state/eV. At the same time, FeNi$_3$ has a sharp band structure near

E_F. The Fermi level falls onto the high-energy slope of the large peak of the DOS (Fig. 1) and the local DOS of a Fe atom at E_F is about 2.7 states/eV·atom [6]. So, there is no "small perturbation" of the electronic structure when we go from pure Fe to $FeNi_3$.

Additionally, at this mass density, the averaged volume per atom for $FeNi_3$ is 7.406 Å^3, whereas it is 7.134 Å^3 for iron, i.e., only by 3.8% smaller. Accordingly, this small difference should cause a difference of the same order in the sound wave results. But, at actual pressures, $FeNi_3$ is more compressible (less stable) because its total DOS near E_F is about 2 times greater than that in iron [4]. So that the electronic contribution to the $FeNi_3$ free energy (Eq. (3)) exceeds that for iron, especially for high temperatures. In other words, with the same averaged volume per atom (7.406 Å^3), the Debye temperature for $FeNi_3$ is about 570 K, whereas it is about 650 K for iron ecause the stiffness of pure Fe is larger than that of $FeNi_3$. Because pure Fe has a smaller mass density than $FeNi_3$ under the same volume per atom, the difference is even more impressing at the same density: at 13 g/cm^3, these values are 570 K for $FeNi_3$ and 700 K for pure iron [8].

Because the outer core does not carry shear waves, the commonly accepted approach is to describe it as a liquid iron alloy. The investigation of the melting process at extreme pressures can give information about the chemical composition, structure, and thermal state of the Earth's core. However, theoretical estimates of the melting temperature of metals are most complicated.

There exists a number of experimental techniques to determine the Debye temperature. The values obtained with different techniques and at different temperatures agree well with each other. For our purpose, the Lindemann law [19] is of particular interest, because it connects the melting point T_m (in K) and the Debye temperature Θ_D (in K) in the following way

$$\Theta_{\rm D} = K\left(\frac{T_m}{M}\right)^{1/2}\frac{1}{\Omega^{1/3}}. \tag{13}$$

Here, M is the mean atomic mass, Ω is the mean atomic volume (in units of cm^3/mol), and K is a phenomenological constant approximately equal to 115. This constant depends to some extent on the chemical composition of the crystal and on the method of determination. In [20], it was pointed out that there is no satisfactory theoretical explanation for this expression, but that it does have an empirical basis. The applicability of the Lindemann law for the estimation of the melting points of transition metals and particularly of iron at extreme pressures was reviewed in [21].

This equation allows us to estimate the melting point of the compound from a theoretical $\Theta_{\rm D}$. However, the value of the Poisson ratio $\sigma \simeq 0.44$ is slightly smaller than its maximum value of 0.5 which belongs either to liquid or to rubber [13]. Apart from that, expression (12) for the Debye temperature contains the multiplier $(1-2\sigma)$. Hence, one may ask to what extent the proposed approach can yield the melting temperatures. With this purpose, the Debye temperatures of some pure metals which have the Poisson ratio $\sigma > 0.42$ at ambient pressure are listed in Table 1 (the data are taken from [22]). The Debye temperatures $\Theta_{\rm D}^E$ are determined from elastic constants at 0 K and at 298 K, while the values of $\Theta_{\rm D}^m$ are calculated [22] from the Lindemann equation for $K = 138.5$ (see Eq. 13). In Table 1, we also present $\Theta_{\rm D}^m$ for $K = 115$. The comparison of $\Theta_{\rm D}^E$ to $\Theta_{\rm D}^m$ suggests that the agreement between them is reasonable, but, for "quasiliquid" metals, a better agreement is achieved using $K = 115$ which we take to estimate the melting point of $FeNi_3$. Athough the inner core is both at extreme pressure and high temperature, the ratio of the temperature to the binding energy for $FeNi_3$ is approximately the same as for the "quasiliquid" metals under normal conditions. Thus, we believe that the Lindemann equation is a fairly good approximation for the Debye temperature for the problem under consideration. So, we may hope that the solution of the inverse problem — the determination of the melting point from the Debye temperature — can provide reliable estimates.

The calculated dependences of the melting point versus the density for three hypothetical temperatures of the inner core are plotted in Fig. 3. The curves differ only slightly because, at the inner core densities, it is the compression of the electron gas that most strongly contributes to the Debye temperature, rather than the thermal excitation of electrons. Fig. 3 reveals a rather small temperature effect on the elasticity characteristics of the compound, which may be due to the fact that we use seismological data for σ. As has been mentioned above, the Poisson ratio is assumed to be temperature-

Table 1. Comparison of the values of the Debye temperature (in K) determined from elastic constants ($\Theta_{\rm D}^E$) and from the Lindemann equation ($\Theta_{\rm D}^m$) for metals with $\sigma \geq 0.4$

Metal	σ	$\Theta_{\rm D}^E$		$\Theta_{\rm D}^m$	
		0 K	298 K	K=138.5	K=130
49 In	0.46	111.3±1.1	85	107	100.4
79 Au	0.425	162	160±4	166	155.8
81 Tl	0.46	—	55	90.1	84.6
82 Pb	0.44	105	81±9	89.5	84.0

independent and equal to the geophysically observed value at the center of the inner core.

It is striking that, at the averaged inner core density of 13 g/cm^3, the theoretically obtained melting temperatures agree fairly well with their geophysical estimates for the Earth's core (3000 — 4000 K) [18] in contrast to those for pure iron, which is (7600±500) K at the inner core — outer core boundary [23]. Additionally, our results agree with those in [24] where it was pointed out that the addition of nickel to iron leads to a melting point depression; the effect increases dramatically with pressure.

Finally, we note that, even by using a more general and precise thermodynamic theory, one could hardly expect to have a better accuracy because of the lack of knowledge of the chemical composition and crystal structure of the inner core.

4. Conclusion

The first-principle electronic structure calculations within LDA have proven to be successful in predicting the elastic properties and equation of state of Fe_3Ni at extreme pressures. Based on our calculations of elastic and thermal properties and relying on PREM [5], we can conclude that crystallographically ordered $FeNi_3$ under the inner core conditions is not elastically as hard as suggested by the PREM. The results of the present work are related rather to the outer core conditions as they are given by PREM. However, as has been often pointed out (see, e.g., [25]), it is for the inner core that the seismic observations provide the least reliable estimates.

In addition, it is obvious that the effect of pressure on the magnetic and elastic properties can depend on even small changes of the chemical composition of the iron-nickel host. Namely, alloying $FeNi_3$ with light element impurities can move the low-spin magnetization peak towards both high or low mass densities. Furthermore, the effect of impurities can tune the distinct peaks of DOS onto the Fermi level, so that it can amplify the magnetization by stabilizing the high-spin ferromagnetism. It is just that was observed from electronic structure calculations [26] of the close packed Fe_3S at Earth's core pressures which additionally reveal a distinct peak in the total DOS near E_F.

The experimental verification of the above theoretical predictions would require measurements of magnetic and elastic properties at megabar pressures. The technique recently proposed in [27] seems to be appropriate for such a task. A realization of appropriate experiments would shed light on such a single-solid-phase model.

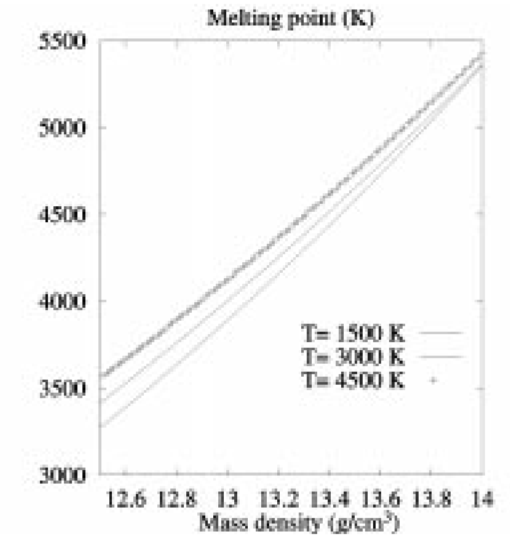

Fig. 3. Calculated melting point of ferromagnetic $FeNi_3$ for three hypothetical temperatures of the inner core

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ПРУЖНІ ТА ТЕРМІЧНІ ВЛАСТИВОСТІ СПЛАВУ $FeNi_3$ В УМОВАХ ВНУТРІШНЬОГО ЯДРА ЗЕМЛІ

О.Є. Красовський

Резюме

Проведено розрахунки електронної будови кристалографічно упорядкованого сплаву $FeNi_3$ при екстремальних тисках та різних температурах. Вивчено пружні та термодинамічні параметри цієї сполуки з метою зіставлення розрахованих значень швидкостей звукових хвиль із спостережуваними величинами швидкостей сейсмічних хвиль, що поширюються у внутрішньому ядрі Землі. Зроблено спробу оцінити температуру плавлення цього сплаву.

УПРУГИЕ И ТЕРМИЧЕСКИЕ СВОЙСТВА СПЛАВА $FeNi_3$ В УСЛОВИЯХ ВНУТРЕННЕГО ЯДРА ЗЕМЛИ

А.Е. Красовский

Резюме

Проведены расчеты электронного строения кристаллографически упорядоченного сплава $FeNi_3$ при экстремальных давлениях и различных температурах. Изучены упругие и термодинамические параметры этого соединения с целью сопоставления рассчитанных значений скоростей звуковых волн с наблюдаемыми величинами скоростей сейсмических волн, распространяющихся во внутреннем ядре Земли. Предпринята попытка оценить температуру плавления этого сплава.