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Electronic Properties of Tetrataenite $L1_0$ FeNi at Earth's Core Conditions

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Physics of Earth's core is crucial to give insight into the origin and behavior of the Earth and other terrestrial planets. In order to interpret the behavior of tetrataenite $L1_0$ FeNi at Earth's inner core boundary and Earth's center conditions, we report electronic properties namely electronic charge density and Fermi surface of tetrataenite $L1_0$ FeNi using the first-principles plane wave self-consistent method under the framework of density functional theory. For structural and electronic properties of tetrataenite $L1_0$ FeNi at the Earth's core conditions, we used spin polarization and ultrasoft pseudopotential with the exchange correlation of Perdew-Burke-Ernzerhof (PBE). Variable cell optimization (VC-relax) calculation using Wentzcovitch dynamics as implemented in Quantum ESPRESSO code is used for estimating equilibrium lattice constant of tetrataenite phase of $L1_0$ FeNi at 0 K. Bonding character between Fe-Fe, Ni-Ni and Fe-Ni metal atoms is discussed at 0 K and extreme Earth's core conditions. The complicated shape of comprehensive Fermi surface is observed which occurred from the merging of all individual Fermi surfaces due to corresponding band crossing at Fermi level E_F in the electronic band structure. Relation between crossing of each band in the electronic band structure with high symmetrical points of the Brillouin zone and the corresponding shape of Fermi surfaces are discussed. Conclusions based on the electronic charge density plot and Fermi surface topology of tetrataenite $L1_0$ FeNi at Earth's core conditions are summarized.

Keywords: Tetrataenite, $L1_0$ FeNi, Earth's core, Electronic charge density, Fermi surface, DFT.

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1. INTRODUCTION

Deep-rooted discussion has perpetuated regarding the nature of the Earth's inner core including its age, composition of its structure and its dynamic behavior at high pressure and high temperature [1]. The precise structure and composition of the Earth's core is still in discussion [2]. Understanding of the core composition and structure is crucial to interpret the seismic data and build a geophysical model [3]. Generally Fe is the primary component of the Earth's inner core, but cosmochemical model and meteorites also suggested the existence of some Ni [2] in the inner core of the Earth. Additional to light elements, the major alloying element in the Earth's inner core is nickel and it is familiar that the inner core of the Earth is composed of Fe with 5-15 wt. % Ni content. Thus, the addition of impurities like Ni is an important factor to modify the phase stability and elastic properties of Fe [4]. Abundant research has been done on Fe-Ni alloys at Earth's core conditions which accord varying results [1-7]. Static Diamond Anvil Cell (DAC) experiments with 10 wt. % Ni in Fe have presumed only the hcp structure up to 340 GPa and 4700 K [5, 6]. Experimental studies with different concentrations of Ni (15, 25 and 32.5 wt. %) favour the fcc structure of Ni, even though light conditions (25 GPa, room temperature) were used [7]. The inclination towards increasing fcc stability with increasing Ni is also reported in quasi-harmonic study on Fe-Ni alloys [2] whereas classical molecular dynamics simulations of Fe-Ni alloys at 6600 K presume that Ni will destabilize the fcc structure with respect to the hcp at 360 GPa [3]. It has been also observed that Ni has minor effect on the elastic properties of Fe and stabilizes the fcc structure up to about 7000 K [4]. Reaman [1] has fixed an equation of state of a planetary-core representative $Fe_{64}Ni_{36}$ (36 wt. % Ni) alloy to 95 GPa and ~ 3000 K, and also predicted that increase in Ni content relative to the estimated abundance in the inner core yields an evaluative study on the effects of increasing Ni proportion on the equation of state of FeNi alloys. The instability of Fe_3Ni with small tetragonal distortions, the Invar behavior, and the LM (low moment) ↔ HM (high moment) transitions are relevant to the intricate balance of charge distribution and magnetic order from *d*-orbital of Fe_3Ni possessing different bonding character [8]. This feature has stimulated us to not restrict our study only up to phonon dispersion and electronic band structure [9] of invar alloys but to enlarge it by exploring the electronic charge density plot. The pitch of oscillations (along p_z) in the anisotropies of the Compton profiles of transition metals is controlled by the Fermi surface topology. In addition, it is well-known that shape and volume of the Fermi surface reflect the electrical properties of metals. Such factors have inspired us to investigate the Fermi surface topology of various Fe-Ni invar alloys using first principles calculations. Gruner et al. [10] have studied the spin-polarized minority spin Fermi surface of Fe_3Ni and concluded that the Kohn anomaly is responsible for the low temperature structural changes in the ordered alloys. Prompting from the work of Gruner et al. [10] and Reaman [1] and thereby providing innate knowledge into the behavior of Fe-Ni alloys at higher pressures and temperatures with appli-

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cations to other planetary cores, we have afforded to investigate the electronic properties namely electronic charge density and Fermi surface of tetrataenite $L1_0$ FeNi (approximately 50 wt. % Ni) having approximately 14 wt. % Ni higher content compared to $Fe_{64}Ni_{36}$ of previous work [1]. By means of first-principles calculations, the present work mainly aims to examine how electronic properties namely electronic charge density and Fermi surfaces of tetrataenite $L1_0$ FeNi are affected by such extreme high temperature and pressure. A lot of research has been done on the magnetic properties of tetrataenite $L1_0$ FeNi. But the scarcity of the mentioned electronic properties of tetrataenite $L1_0$ FeNi at high temperature/pressure nearer to Earth's core conditions has encouraged us for the present investigations. The paper is organized as follows. The next section 2 describes computational methodology used in the present study. The section 3 presents the results and discussion. Section 4 concludes the results.

2. COMPUTATIONAL METHODOLOGY

The only structure of FeNi consistent with X-ray and Mossbauer results is the $L1_0$ (CuAu) structure [11]. This tetragonal structure can be obtained from the face-centered taenite structure by arranging Fe and Ni atoms on alternate (002) planes [11]. Tetrataenite unit cell of FeNi exhibit two atom basis Fe (0, 0, 0) and Ni (1/2, 1/2, 1/2). Structural properties of tetrataenite $L1_0$ FeNi are computed using plane wave pseudopotential density functional theory (DFT) within generalized gradient approximation (GGA) as implemented in Quantum ESPRESSO code [12].

For structural and electronic properties of $L1_0$ FeNi at Earth's core conditions, we used spin polarization and ultrasoft pseudopotential with the exchange correlation of Perdew-Burke-Ernzerhof (PBE) [13]. Variable cell optimization (VC-relax) calculation using Wentzcovitch dynamics as implemented in Quantum ESPRESSO code [12] was used for estimating equilibrium lattice constant of tetrataenite phase of $L1_0$ FeNi at 0 K. In order to estimate equilibrium lattice constant of tetrataenite phase of $L1_0$ FeNi at Earth's core conditions, we used the experimentally available cell parameters $a = 2.53$ Å and $c/a = 1.414$ [11, 14] and our computed cell parameters $a = 2.58$ Å and $c/a = 1.323$ [9], and atomic positions at 0 K [15] as a starting point and then obtained the equilibrium lattice constant (for fixed experimental $c/a = 1.414$ and our computed $c/a = 1.323$) at Earth's core conditions by using quasi-harmonic Debye model implemented in pseudo code Gibbs [16]. Detail methodology is available in previous published work [9].

Further to study the bonding characterization and charge distribution, we have calculated the charge density plot of tetrataenite $L1_0$ FeNi in diagonal plane using the methodology described in Quantum ESPRESSO [12].

The behavior of the electronic bands crossing the Fermi level E_F from the valence band to the conduction band or from the conduction band to the valence band can be explained in depth from the visualization of Fermi surfaces of the metallic or half-metallic alloys. Hence we have obtained the Fermi surface topology (for each band crossing the Fermi level E_F and merge bands) by using the detailed methodology given in the PWSCF Quantum ESPRESSO [12].

3. RESULTS AND DISCUSSION

Present work summarized the computation of structural and electronic properties of tetrataenite $L1_0$ FeNi at the extreme Earth's core conditions. Equilibrium lattice constant a and ratio c/a of tetrataenite $L1_0$ FeNi at 0 K [15] are computed using variable cell optimization (VC-relax) and are reported in our previous work [9]. Variable cell optimization of tetrataenite $L1_0$ FeNi relaxed with total force of $1 \cdot 10^{-5}$ Ry/a.u., which is sufficient for minimum energy configuration.

To investigate the bonding nature and charge distribution, the analysis of electronic charge density plot is essential. The electronic charge density plot of tetrataenite $L1_0$ FeNi at 0 K in the diagonal plane is shown in Fig. 1. From Fig. 1 it is clearly seen that more charges are accumulated surrounding Ni metal atom, while the presence of green color between Fe and Ni metals predicts metallic bonding between Fe and Ni. Fig. 1 depicts the charge density of tetrataenite $L1_0$ FeNi along the diagonal plane where the two nearest Fe-Fe metal atoms are connected through the green color between them, which predicts metallic bonding between nearest Fe-Fe metal atoms.

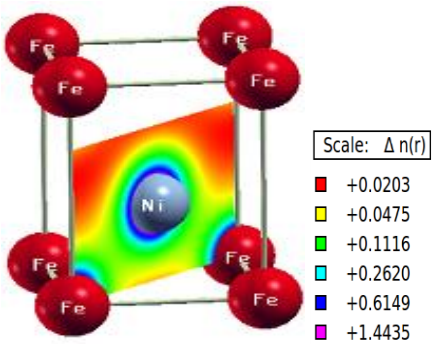

Fig. 1 – (color online) Total charge density plot of tetra-taenite $L1_0$ FeNi at 0 K along the diagonal plane. Charge densities are in arbitrary units. Color-code scale is displayed in the figures

To understand the influence of extreme temperature and pressure on bonding nature of Fe and Ni in tetrataenite $L1_0$ FeNi, the present study shows the investigation of the charge density plot at extreme temperature and pressure of Earth's core.

It is well-known that, the major compound element in the Earth's inner core is nickel and it is familiar that the inner core of the Earth can be composed of Fe with 5-15 wt. % Ni content. In order to check the behavior of tetrataenite $L1_0$ FeNi (nearly 50 wt. % Ni) at Earth's core conditions, we have computed the charge density of tetrataenite $L1_0$ FeNi at Earth's inner core boundary conditions (330 GPa and 5500 K) and at Earth's centre conditions (360 GPa and 6000 K) for experimentally available cell parameters $a = 2.53$ Å and $c/a = 1.414$ [9] in Fig. 2a and Fig. 2b, respectively. Fig. 2a and Fig. 2b indicate strong metallic bonding between Fe and Ni metal atoms compared to between two nearest Fe metal atoms. Comparison of the charge density plots of Fig. 2a

and Fig. 2b allows to suggest extremely small or even negligible increase in the delocalized electrons between Fe and Ni as moving from Earth's inner core boundary conditions (330 GPa and 5500 K) to Earth's centre conditions (360 GPa and 6000 K) which is in agreement with the previously reported electronic band structure of tetrataenite L1$_0$ FeNi [9], in which electrons occupy slightly higher energy as moving from Earth's inner core boundary to its centre. Comparing presently reported charge density plots of tetrataenite L1$_0$ FeNi at the Earth's core conditions with that of tetrataenite at 0 K (Fig. 1), it can be said that tetrataenite L1$_0$ FeNi occupies slightly higher charge density at Earth's core conditions compared to that at the condition of 0 K.

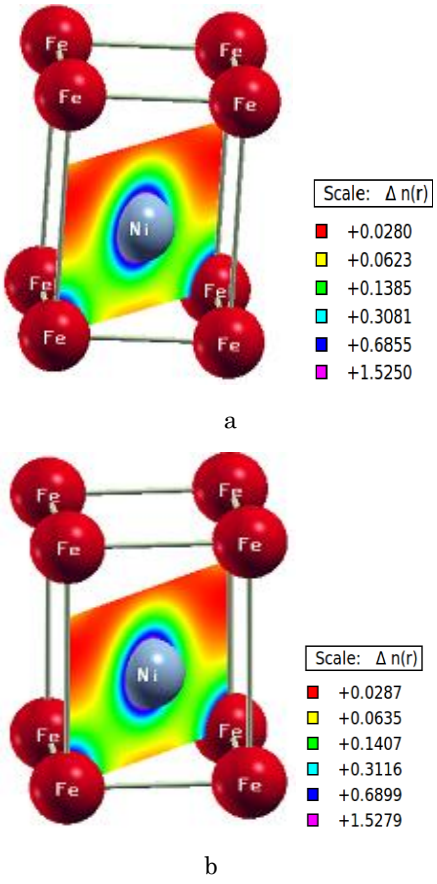

Fig. 2 – (color online) (a) Total charge density plot of tetrataenite L1$_0$ FeNi at Earth's inner core boundary conditions along the diagonal plane; (b) total charge density plot of tetrataenite L1$_0$ FeNi at Earth's centre conditions along the diagonal plane. Charge densities are in arbitrary units. Color-code scale is displayed in the figures

The surface having constant energy E_F in k space is called Fermi surface which splits the unfilled orbitals from the filled orbitals, at absolute zero. In other words, it is the surface in momentum space where, in the limit of non-interactions, all fermions' states with momentum $k < k_F$ are filled, and other higher momentum states are unfilled.

Any changes in the occupancy of states near the Fermi surface can generate the electrical current and hence the shape and volume of the Fermi surface are useful to measure the electrical properties of the metals. Fermi surface is the place where all the bottommost excitations of the systems live. For room temperature experiments, Fermi energy is larger than room temperature and hence whole thermodynamics of the material is controlled by excitations occurring at the Fermi surface. Thus, the thermodynamic properties of the material can be known by the concept of Fermi surface.

In the previous study [9], the electronic band structure and DOS of tetrataenite L1$_0$ FeNi are computed in which the results of DOS show deep valley i.e. a pseudogap right at the Fermi level which is a symptom of severe redistribution of states [10]. This evidence has encouraged for detailed study of Fermi surfaces of tetrataenite L1$_0$ FeNi.

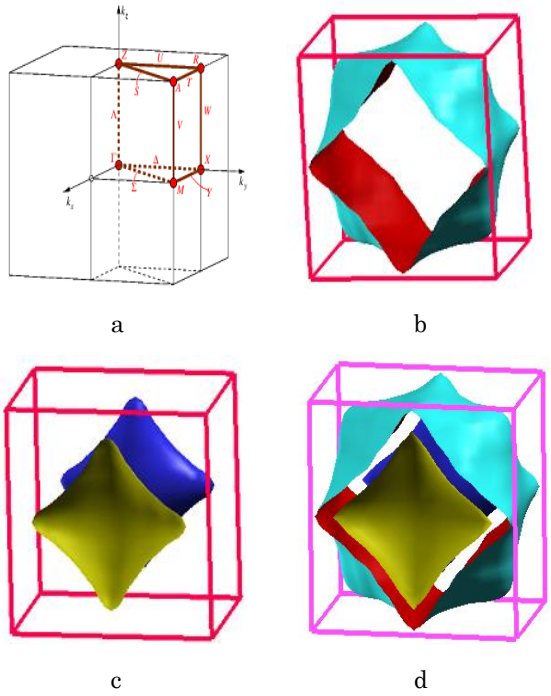

Fig. 3 – (color online) (a) Standard shape of Brillouin zone for tetrataenite L1$_0$ phase with unit cell space group P4/mmm (123) obtained from ref. [17]; (b), (c) Fermi surfaces of tetrataenite L1$_0$ FeNi at 0 K for each individual band crossing the Fermi level for spin up states and (d) Fermi surface of tetrataenite L1$_0$ FeNi for merging of all bands crossing the Fermi level for spin up state

In order to understand the electrical properties of tetrataenite L1$_0$ FeNi, we have computed the Fermi surfaces at 0 K and extreme Earth's core conditions within the framework of DFT as implemented in Quantum ESPRESSO code.

Fig. 3a shows the typical shape of Brillouin zone for tetrataenite L1$_0$ phase with unit cell space group P4/mmm (123) as obtained in ref. [17]. Figs. 3b, c, d display the Fermi surface topology of tetrataenite L1$_0$ FeNi for spin up states. From Fig. 3b it can be seen that the Fermi surface topology exhibits hole character at M-point and is well supported by band structure of Fig. 4a [9]. Fig. 3c indicates two electron-like Fermi surface sheets towards YZ plane of the Brillouin zone [18]. Fig. 3d displays the comprehensive Fermi surface topology of tetrataenite L1$_0$ FeNi for spin up states.

Figs. 5a, b, c indicate the Fermi surface topology of tetrataenite L1$_0$ FeNi for spin down states where three

Fermi surfaces appear due to the crossing of three bands at the Fermi level E_F. By comparing the Fermi surfaces of spin down states with the band structure of Fig. 4b [9], it can be seen that the Fermi surface in Fig. 5c is due to the single band crossing at X-point, Γ-point and along Γ-A directions [18]. Fermi surface topology of tetrataenite $L1_0$ FeNi for spin down states is evidenced by the band structure of Fig. 4b.

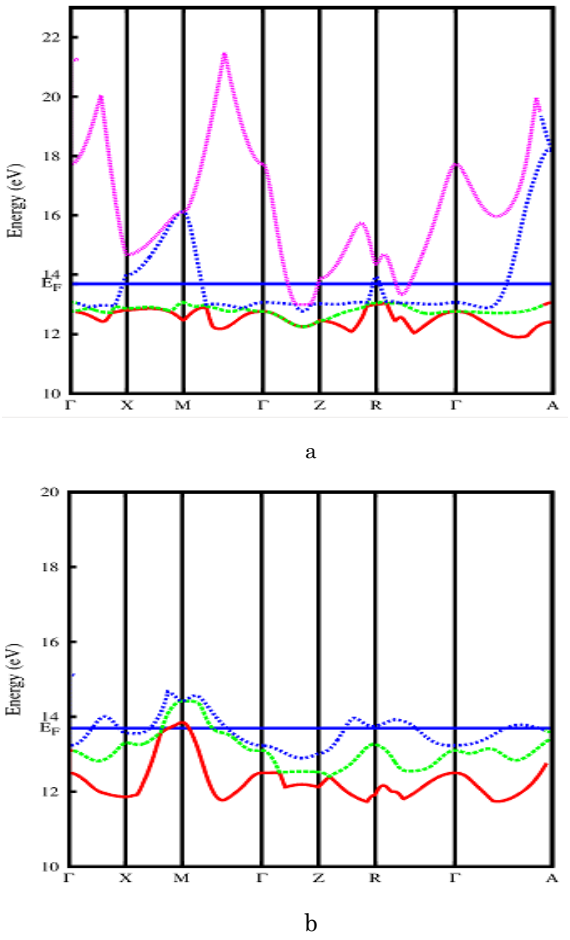

Fig. 4 – (color online) Electronic band structure of tetrataenite $L1_0$ FeNi only for the bands crossing the E_F: spin up directions (a) and spin down directions (b) [9]

Fig. 6 and Fig. 7 indicate the Fermi surface topology of tetrataenite $L1_0$ FeNi at Earth's inner core boundary conditions (330 GPa and 5500 K) for spin up and spin down states, respectively. In Fig. 6, Fermi surfaces occur due to the corresponding significant crossing of bands for the spin up states. In Fig. 7b, the Fermi surface topology for spin down states exhibits significant portion along Γ, Z, M and R directions which is due to the significant crossing of bands along these directions in the corresponding electronic band structure [9]. Other topology of Fermi surface for spin down states in Fig. 7c is similar to that observed at extreme conditions of high temperature and pressure for spin up states.

Figs.8a, b, c indicate the Fermi surface topology of tetrataenite $L1_0$ FeNi at Earth center conditions (360 GPa and 6000 K) for spin up states, while Fig. 8d displays the topology of the Fermi surface for spin down electrons.

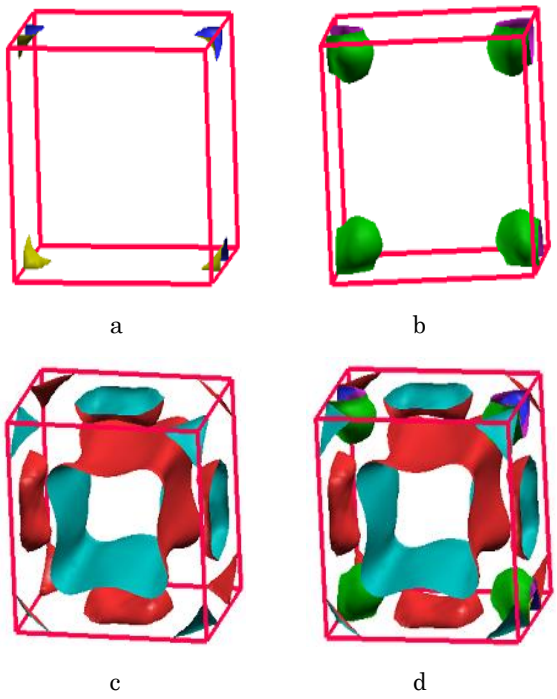

Fig. 5 – (color online) (a-c) Fermi surfaces of tetrataenite $L1_0$ FeNi at 0 K for each individual band crossing the Fermi level for spin down states; (d) comprehensive Fermi surface of tetrataenite $L1_0$ FeNi for spin down states

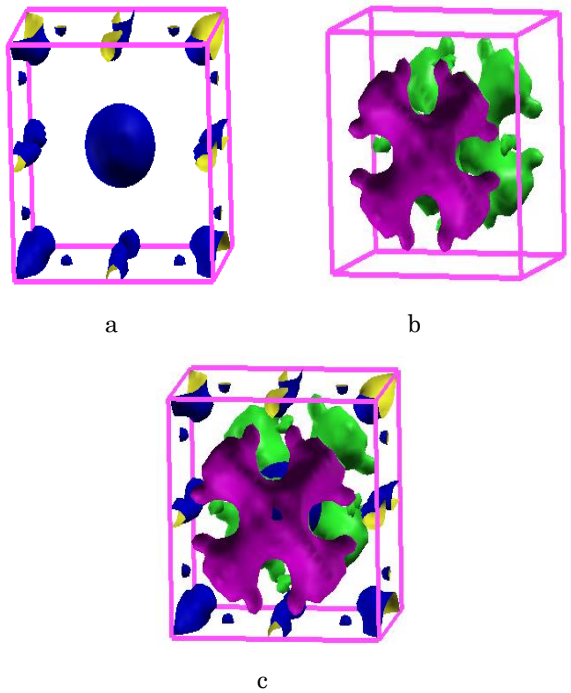

Fig. 6 – (color online) (a, b) Fermi surfaces of tetrataenite $L1_0$ FeNi at Earth's inner core boundary conditions for each individual band crossing the Fermi level for spin up states, (c) Fermi surface of tetrataenite $L1_0$ FeNi at Earth's inner core boundary conditions for merging of all bands crossing the Fermi level for spin up states

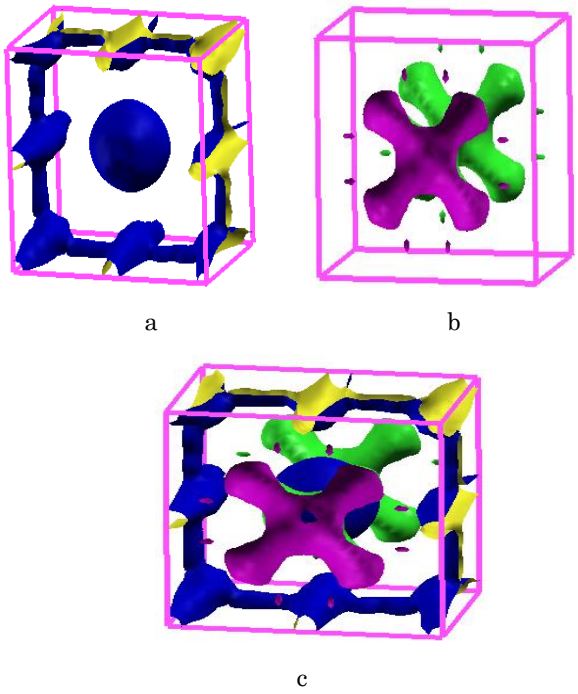

Fig. 7 – (color online) (a, b) Fermi surfaces of tetrataenite $L1_0$ FeNi at Earth's inner core boundary conditions for each individual band crossing the Fermi level for spin down states, (c) Fermi surface of tetrataenite $L1_0$ FeNi at Earth's inner core boundary conditions for merging of all bands crossing the Fermi level for spin down states

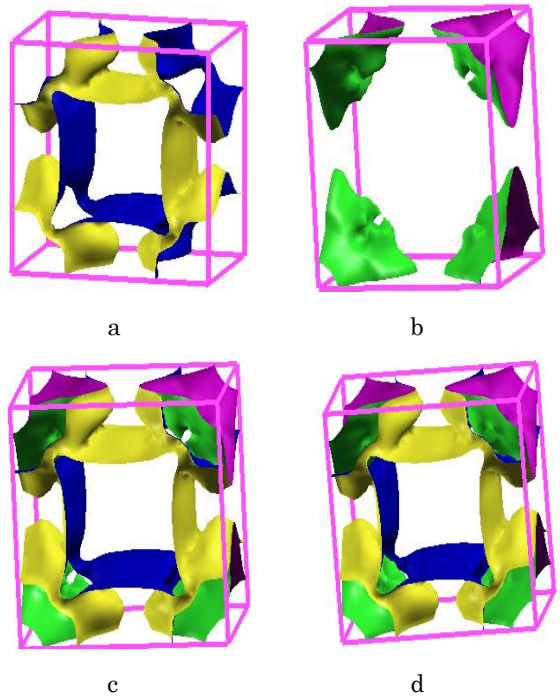

Fig. 8 – (color online) (a, b) Fermi surfaces of tetrataenite $L1_0$ FeNi at Earth's centre conditions for each individual band crossing the Fermi level for spin up states; (c) comprehensive Fermi surface of tetrataenite $L1_0$ FeNi at Earth's centre conditions for spin up states, and (d) comprehensive Fermi surface of tetrataenite $L1_0$ FeNi at Earth's centre conditions for spin down states

It is seen that at Earth's centre conditions, topology of the Fermi surface is open Fermi surfaces around Γ-point due to significant crossing along the R-Γ direction followed by extending out towards R-point of the Brillouin zone as shown in Figs.8b, d. Fig. 8b indicates significant Fermi surface at R-point of the Brillouin zone. The Fermi surface topology for spin down states, i.e. Fig. 8d, is equivalent to that for the spin up states as shown in Fig. 8c.

Hence from the analysis of Fermi surfaces of tetrataenite $L1_0$ FeNi at Earth's inner core boundary conditions (330 GPa and 5500 K) and Earth's center conditions (360 GPa and 6000 K), it is concluded that significant shape of the Fermi surface along the *M* and *Z* directions for Earth's inner core boundary conditions (330 GPa and 5500 K) is disappeared for Earth's center conditions as moving from Earth's inner core boundary to Earth's center.

4. CONCLUSIONS

Present paper mainly focuses on detailed investigations on electronic properties of tetrataenite $L1_0$ FeNi which serve useful data for comparison. As both Fe and Ni are well known ferromagnetic transition metals, the combination of Fe and Ni, i.e. Fe-Ni Invar alloys, exhibits complex magnetic behavior. Such magnetic behavior in magnetic materials is ruled by interrelation between the electrons and is well understood by their spin-polarized electronic structure [19]. In addition, complicated balance of charge distribution and different bonding character are crucial for understanding the Invar behavior and low moment to high moment transition in few Invar systems like Fe_3Ni [8]. The charge density plots for tetrataenite $L1_0$ FeNi predict comparatively strong metallic bonding between Fe and Ni compared to between Fe-Fe metal atoms and is well supported by the hybridization of Fe and Ni metal atoms in the previously reported [9] PDOS tetrataenite $L1_0$ FeNi. The investigations of charge density plot of tetrataenite $L1_0$ FeNi at Earth's core conditions conclude that tetrataenite exhibits slightly more charge density at Earth's core conditions compared to that at 0 K. An extremely small increase in the delocalized electrons between Fe and Ni as moving from Earth's inner core boundary conditions (330 GPa and 5500 K) to Earth's centre conditions (360 GPa and 6000 K) is observed which is in agreement with the electronic band structure of tetrataenite $L1_0$ FeNi [9].

The complicated shape of comprehensive Fermi surfaces is observed which occurred from the merging of all individual Fermi surfaces due to corresponding band crossing at Fermi level E_F in the electronic band structure. Fermi surface topology exhibits electron character and/or hole character at different high symmetrical points of the Brillouin zone based on the crossing of bands at E_F in the electronic band structure. Fermi surface along the *M* and *Z* directions for Earth's inner core boundary conditions (330 GPa and 5500 K) is changed significantly and disappeared for Earth's center conditions as moving from Earth's inner core boundary to Earth's center conditions. In the absence of rigorous data on Fermi surface topology of various Fe-Ni phases taken into consideration, it is not possible to compare the results with the other findings.

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Електронні властивості тетратеніту $L1_0$ FeNi в умовах земного ядра

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Фізика ядра Землі має вирішальне значення для розуміння походження та поведінки Землі та інших планет земної групи. З метою інтерпретації поведінки тетратеніту $L1_0$ FeNi на межі внутрішнього ядра Землі та в умовах центру Землі, ми повідомляємо про електронні властивості, а саме електронну густину заряду та поверхню Фермі тетратеніту $L1_0$ FeNi, використовуючи першопринципний самоузгоджений метод плоскої хвилі в рамках функціональної теорії густини (DFT). Для структурних та електронних властивостей тетратеніту $L1_0$ FeNi в умовах земного ядра ми використовували спінову поляризацію та ультрам'який псевдопотенціал з обмінним співвідношенням Пердью-Бьорка-Ернзергофа (PBE). Розрахунок змінної клітинної оптимізації (VC-relax) за допомогою динаміки Венцковича, реалізованої у квантовому коді ESPRESSO, використовується для оцінки рівноважного параметру решітки тетратенітової фази $L1_0$ FeNi при 0 K. Характер зв'язку між атомами металів Fe-Fe, Ni-Ni та Fe-Ni обговорюються для випадку 0 K та екстремальних умов земного ядра. Спостерігається складна форма універсальної поверхні Фермі, яка виникла в результаті злиття усіх окремих поверхонь Фермі за рахунок відповідного перетину смуг на рівні Фермі E_F у структурі електронних смуг. Обговорюється взаємозв'язок між перетином кожної смуги в електронній структурі смуг з високими симетричними точками зони Бріллюена та відповідною формою поверхонь Фермі. Узагальнено висновки на основі графіку електронної щільності заряду та топології поверхні Фермі тетратеніту $L1_0$ FeNi в основних умовах Землі.

Ключові слова: Тетратеніт, $L1_0$ FeNi, Ядро Землі, Електронна густина заряду, Поверхня Фермі, Функціональна теорія густини (DFT).