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

N.Y. Pandya[1,*], Adwait D. Mevada[2], P.N. Gajjar[3,†]

[1] *Parul University, P.O. Limda, Ta. Waghodia, Vadodara, 391760 Gujarat, India*
[2] *President Science College, Ghatlodia, Ahmedabad, 380061 Gujarat, India*
[3] *Department of Physics, University School of Sciences, Gujarat University, Ahmedabad, 380009 Gujarat, India*

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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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