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通过第一性原理预测内地核的成分与结构

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摘要：

内地核成分与结构的确定一直是地球深部研究的重要课题。目前地核的公认成分是铁和少量的镍。但由于地核密度低于纯粹的铁镍合金(固态内核2%~3%,液态外核6%~7%),其中必定掺杂有一定量的轻元素,其种类与浓度有待确定。除成分外,地核条件下铁的晶体结构也有争议。根据地震学观测,声波沿地轴方向的传播速度比赤道平面方向快大约3%~4%。这意味着内地核是各向异性的; 但在极端高压下,晶体构中的原子应该按致密的密排六方结构(h.c.p)排列,而h.c.p结构对声波传输是高度各向同性的,这就需要确定地核条件下铁的晶体结构。根第一性原理计算得到的高压下体系能量以及爱因斯坦谐振子模型,本项研究估算了给定结构的自由能以及掺杂轻元素后的影响。根据计算结可以定性的分析得出,在高压0K下致密的h.c.p结构显然比疏松的体心立方(b.c.c)更稳定; 而随着温度的升高,原子核的振动造成b.c.c结构的由能比h.c.p结构下降得更快,因此在高温下b.c.c结构更稳定; 掺杂轻元素后,这种优势变得更加明显,而3.6at.%的Si则恰好同时解释了2%3%的密度缺失和b.c.c结构在内地核条件下的稳定性。因此我们建议内地核的基本结构与成分应为以体心立方结构存在的铁,掺杂约3.6at.的硅元素,内地核温度至少在5500K以上。这一结论与其它更复杂的方法得到的结果一致。

英文摘要：

The determination of the composition and structure of the Earth's inner core has long been the major subject in he study of the Earth's deep interior. It's widely believed that the Earth's core is formed by iron with a fraction of ni el. However, light elements must exist in the inner core because the earth core is less dense than pure iron-nickel a oy (2%~3% in the solid inner core and 6%~7% in the liquid outer core). The questions are what and how much ligh element is there in the iron-nickel alloy. Besides the composition, the crystal structure of the iron with or without lig element is also not well known. According to the seismological observations, the sound waves propagate 3%~4% ter along the spin axis than in the equatorial plane. That means the inner core is anisotropic. The densest structure f iron-nickel alloy should be h.c.p structure under the very high pressures. However, the h.c.p structure does not pr agate waves anisotropic ally. Then what is the structure of the iron-nickel alloy or the iron-nickle-light element alloy n this study, we tried to predict the composition and the structure of the inner core through ab initio calculation of t Gibbs free energy, which is a function of internal energy, density and entropy. We conclude that the h.c.p structure more stable than the b.c.c structure under high pressure and 0 K, but with the increase of temperature, the free er gy of the b.c.c structure is decreasing much faster than the h.c.p structure caused by the vibration of the atomics, s he b.c.c structure is more stable at high temperatures. With the addition of light elements (S or Si or both), the free nergy of b.c.c. decreases even faster, about 3at% of Si not only explains why the inner core is about 2%~3 % light than the iron-nickle alloy, but also reasons why the inner core is anisotropic, since the b.c.c. structure becomes mor stable than the h.c.p structure at 5500~6000K and b.c.c. is anisotropic in propagating seismic waves. Therefore, w nfer that the inner core of the earth is formed by b.c.c iron and a fraction of nickel plus ~3.6at.% Si, with a tempera e higher than 5500K, which is consistent with the studies from other approaches.

关键词：地球深部 内地核 第一性原理 内地核成分 内地核结构

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