The equation of states of B2 and bcc $Fe_{1-x}Si_x$

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The Earth's inner core is thought to be a Fe alloy containing Ni and several percent of light elements (e.g., Birch 1952). Si is one of the candidates for the light elements. In a Fe-Si system with a large amount of Si, the cubic phases—B2 or body-centered cubic(bcc) structure—become stable at high temperatures and pressures (Fischer et al. 2013, Ikuta et al. 2021). In B2 FeSi, Fe and Si atoms occupy the (0, 0, 0) and (1/2, 1/2, 1/2) sites, respectively. In contrast, the bcc FeSi has Fe and Si atoms occupying these two sites randomly. Since the transition between the ordered B2 and the disordered bcc structure is a second order, the degree of the disorder can change continuously. In the previous experiments, the phase was identified by X-ray diffraction lines from the 001 and 111 planes, which are characteristic of the B2 structure. However, these diffraction lines do not disappear unless the phase is completely transformed to the bcc phase. The B2 phase can have a finite degree of disorder. In this study, we combined the Korringa-Kohn-Rostoker (KKR) method with the coherent potential approximation (CPA) to compute the equation of state of $Fe_{1-x}Si_x$ with B2 and bcc structures. This may lead to a discussion of the phase transition temperature between the two structures by comparing the Gibbs energies.
The total energies of the B2, bcc, and their intermediate structures were calculated for compositions of $Fe_{1-x}Si_x$ (x =0, 0.1, 0.2, 0.3, 0.4, and 0.5). The Kohn-Sham equation was solved by the KKR method (Akai 1989). The chemical disorder was represented within the CPA. The volume range was set to 75-200 $Bohr^3$ (11.11-29.64 $Å^3$). The PBE-type generalized gradient approximation was used for the exchange-correlation functional (Perdew et al. 1996). Both spin-polarized and non-spin-polarized calculations were performed. The obtained total energies were fitted to the third-order Birch-Murnaghan equation of states.
First, we confirmed that the calculated results for the end-member compositions (x = 0 and 0.5) reproduced the previous experimental results. The calculated results of the ferromagnetic Fe are in good agreement with the experiments of Jephcoat et al. (1986), and the results of the non-magnetic B2 FeSi are consistent with Sata et al. (2010). Next, we examined the effects of composition, magnetism, and chemical disorder on the lattice volume. For the effect of composition, the volumes of the non-magnetic B2 phases tend to increase with increasing Fe concentration. For the effect of magnetism, the volumes of the ferromagnetic phase were larger than the non-magnetic phases. For the effect of chemical disorder, the volume of bcc phases were larger than that of the B2 phase. Finally, we discuss the Si concentration, assuming that the inner core is B2 or bcc $Fe_{1-x}Si_x$ single phase. We calculated the pressure and bulk sound velocity from the present equation of states at the density corresponding to the inner core. As a result, we found that both pressure and bulk sound velocity increase with increasing Si concentration. Note that the equation of states are obtained at zero Kelvin. In general, the pressure is expected to increase and the bulk sound velocity decrease with increasing temperature. The pressures and the bulk sound velocities obtained in this study were compared with the Preliminary reference Earth model (PREM) (Dziewonski and Anderson 1981), one of the Earth's internal structure models. The calculated pressure for $Fe_{0.8}Si_{0.2}$ at the inner core density was higher than the PREM value. Thus, pressure imposes a constraint of $x < 0.2$ on the inner core composition. Similarly, the bulk sound velocity of $Fe_{0.9}Si_{0.1}$ is lower than the PREM, imposing $x > 0.1$. Therefore, if the inner core consists of B2 or bcc $Fe_{1-x}Si_x$ single phase, the inner core composition is considered to be between $Fe_{0.9}Si_{0.1}$ and $Fe_{0.8}Si_{0.2}$.

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