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Equilibrium iron stable isotope fractionation at core-mantle boundary conditions.

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Resent iron stable isotope studies showed that Lunar and Eath mantle samples are abundant in the heavy isotope relatively to samples from Mars, Vesta and primitive undifferentiated meteorites, chondrites (Poitrasson et al.. 2004; Weyer et al., 2005, Schoenberg and von Blanckenburg, 2006, Williams et al. 2006). Different explanations of this observation were discussed in literature (e.g. Poitrasson, 2007; Weyer et al., 2007; Beard and Johnson, 2007). Two alternative mechanisms of iron isotope fractionation leading to the abundance of Lunar and Earth mantle samples in heavy iron isotopes were proposed: 1) the abundance in heavy iron isotope is caused by the accretion specificity; 2) the abundance is resulted from stable isotope fractionation during mantle-core differentiation.

Georg et al. (2007) tried to estimate the iron isotope fractionation resulted from the disproportionation of iron ($3Fe^{2+} \leftrightarrow 3Fe^{2+} + Fe^0$) during core formation. For this purpose, they estimated equilibrium iron isotope fractionation between metallic iron and two major oxide component of the low mantle, ironpericlase ($Fe_xMg_{1-x}O$) and ironperovskite ($Fe_xMg_{1-x}SiO_3$). Georg et al. (2007) conducted their calculation using the equilibrium iron isotope fractionation factors (β-factors) obtained by Polyakov and Mineev (2007) from Moessbauer spectroscopy data at pressure 1 bar. As it is shown in the present study, iron β-factors for the low-mantle minerals increase with pressure dramatically. Having no data on the iron β-factor for perovskite, Georg et al. (2007) used the iron β-factor for hematite instead of that for perovskite. For these reasons the estimation of the iron isotope fractionation during mantle-core differentiation presented by Georg et al. (2007) cannot be accepted without reservations.

In this study, I used the new method of calculation iron β-factors from data on inelastic nuclear resonant Xray scattering (INRXS) in synchrotron radiation experiments (Polyakov et al., 2005, 2007). This method requires knowledge of the phonon density of states (DOS) for at least two isotopologues. This method used the partial DOS referring to the iron sublattice which can be obtained by INRXS experiments. Combining the INRXS and the diamond anvil one can obtain the DOS of iron subblatice at high pressures and use it in calculations of the β-factors at high pressures. I used the partial DOS of metallic iron, ironpericlase ($Fe_{0.25}Mg_{0.75}O$) and postperovskite ($Fe_{0.4}Mg_{0.6}SiO_3)$ obtained at pressure up to 130GPa by Mao et al. (2001) and (2006) and by Lin et al. (2006) in my calculations of β-factors. I also used McCammon (1998) data on the second-order Doppler shift in the Moessbauer spectra of perovskite ($Fe_{0.05}Mg_{0.95}SiO_3)$ to estimate the iron β-factor for perovskite.

As it follows from my calculations, values of lnβ for iron isotope fractionation at mantle-core boundary pressures are from 2.0 to 4 times higher than those at ambient pressure. For example, at room temperature for metallic iron, 10^3lnβ is about 8.1 at ambient pressure and about 19.9 at 112 Gpa for $^{57/54}$Fe fractionation. For ironpericlase, the same values are 7.8 at ambient pressures and 20.1 at 109 GPa. These changes in the β-factors values result in appropriate changes in iron isotope fractionation coefficients which are related by simple equation:

$10^3\ln\alpha_{A-B} = 10^3\ln\beta_A - 10^3\ln\beta_B$
where α_{A-B} is the isotope fractionation coefficient between A and B phases; β_A and β_B are the β-factors of A and B phases, respectively.

Magnitude of equilibrium iron isotope fractionation coefficient between (post)perovskite and metallic iron at 130 GPa exceeds that between perovskite and metallic iron at ambient pressure significantly (Equilibrium iron isotope fractionation coefficient between (post)perovskite and metallic iron at 130 GPa is about 5 time higher than that between hematite and metallic iron at ambient pressure. The latter was used by Georg et al. (2007) instead of iron isotope fractionation coefficient between perovskite and metallic iron). If should be also stressed that equilibrium iron isotope fractionation coefficients between (post)perovskite and metallic iron at 130 GPa and that between perovskite and metallic iron at have different signs. $^{57/54}$Fe isotope fractionation coefficient between (post)perovskite and metallic iron at 130 GPa ranges from 0.2 to 0.05$\%_¸$ at temperatures from 2000 to 4000 K. Our estimation for the ironpericlase – metallic iron isotope fractionation coefficient gives value that are very close to zero at high P – high T conditions. Finally, our study gives values from 0.025 to 0.1$\%_¸$ for $^{57/54}$Fe fractionation between mantle and core. We took into account that a half of iron atoms are in the low mantle periclase phase according to the estimate by Kesson et al., 1998.

It should be noted that one can expect abundances of the silicate phase in light iron isotope at low pressures. This is in agreement with observations for iron meteorites and pallasites (Poitrasson 2007).

Based on present calculations, one can conclude that iron isotope fractionation during mantle-core differentiation may be probable mechanism resulting in the abundance of Lunnar and Earth mantle samples in heavy iron isotope.