

Equilibrium carbon isotope fractionations between silicate melts and iron melts

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The carbon budget in the Earth interior is currently not well constrained. How and when carbon was delivered to the Earth is also an open question. The timing of carbon delivery to the Earth has different consequences. We report here the first theoretical calculation study on equilibrium carbon isotope fractionations between silicate melts and iron melts at the pressures of 0, 40, 80 and 120 GPa and at various redox conditions, using first-principles methods. Previous studies used crystalline analogues to represent melts instead of melt itself in isotope fractionation calculations. Our results suggest that iron melt is significantly depleted in ¹³C relative to silicate melt even at the temperatures of planetary core formation. The carbon isotope fractionation increases with increasing oxidation degree of silicate melt. The pressure effect on carbon isotope fractionation cannot not be ignored and its direction and magnitude strongly depend on the redox condition. Consequently, the fractionation factors of ¹³C/¹²C measured from low pressure experiments may not be applicable to isotope fractionations during Earth's core formation which occurred at much higher pressure. Equilibrium carbon isotope fractionations among magnesite (MgCO₃), diamond, moissanite (SiC) and various iron-carbides are distinctly different from those of melts. Thus, defective conclusions may be obtained when predicting the carbon isotope fractionation between mantle-forming silicate melt and core-forming metal melt based on the theoretical calculations on crystalline compounds.

The calculated carbon isotope fractionations, which are under the bottom conditions of proto-Earth's magma ocean, cannot compromise the equilibrium or Rayleigh distillation isotope fractionation way of Earth's core segregation and lead to a strange carbon isotope signal of the mantle (i.e., around -7.2 per mil). However, it can be explained by the core segregation of other much smaller planetary embryos, rather than that of Earth. We suggest that the delivery agent of BSE's major carbon may be a Mars-like body. We also use SPH- and MFM-based simulations to find out conditions required for such core-core merge giant impacts.