Experimental determination of carbon diffusion in liquid iron at high pressure ANNA M. REBAZA^{1,2,3}, ESTHER S. POSNER^{1,*}, MARCEL THIELMANN¹, DAVID C. RUBIE¹, AND GERD STEINLE-NEUMANN¹

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ABSTRACT

The transport properties of liquid iron alloys at high pressure (P) and temperature (T) are essential for understanding the formation, composition, and evolution of planetary cores. Light alloying elements (e.g., Si, O, S, C, N, H) in liquid iron are particularly relevant due to the density deficit of Earth's core, yet high P-T experimental diffusion studies involving such alloys remain scarce, with large uncertainties on the P and T dependence required for extrapolation to core conditions. In this study, we measured the chemical diffusion of carbon in liquid iron over a P-T range of 3-15 GPa and 1700-2450 K using a multi-anvil apparatus. Diffusion couples consisting of pure Fe and Fe-2.5 wt%C cylinders were placed end-to-end in an MgO capsule in a vertical orientation. Carbon concentration profiles were measured by electron microprobe and modeled numerically to correct for non-isothermal diffusion that occurred prior to reaching the peak temperature. Carbon diffusion coefficients range from $6 \times 10^{-9} \text{ m}^2 \cdot \text{s}^{-1}$ to $2 \times 10^{-8} \text{ m}^2 \cdot \text{s}^{-1}$, with global Arrhenian fit parameters $D_0 = 1.4 \pm 0.5 \times 10^{-7} \text{ m}^2 \cdot \text{s}^{-1}$, $\Delta E = 43 \pm 6 \text{ kJ/mol}$, and $\Delta V = -0.06 \pm 0.19$ cm³·mol⁻¹. A negligible P effect is consistent with previous studies of oxygen diffusion in liquid iron and high-T calculations but differs from larger ΔV values previously reported from carbon self-diffusion experiments for liquid Fe₃C and simulations for an Fe-Ni-C alloy. Carbon diffusion coefficients determined here are approximately three times faster than those reported from Fe-Ni-C liquid simulations, which highlights the potential significance of compositional effects on mass transport properties of liquid iron alloys and the need for expanding the P-T experimental diffusion data set currently available in the literature to more complex and geologically relevant compositions.

Keywords: Carbon diffusion, core formation, outer core, liquid iron alloys, interstitial alloys