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Density determination of liquid iron-nickel-sulfur at high pressure

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Abstract

The density of liquid iron-nickel-sulfur ($Fe_{46.5}Ni_{28.5}S_{25}$) alloy was determined at pressures up to 74 GPa and an average temperature of 3400 K via pair distribution function (PDF) analysis of synchrotron X-ray diffraction (XRD) data obtained using laser-heated diamond-anvil cells. The determined density of liquid $Fe_{46.5}Ni_{28.5}S_{25}$ at 74 GPa and 3400 K is 8.03(35) g/cm^3, 15% lower than that of pure liquid Fe. The obtained density data were fitted to a third-order Vinet equation of state (EoS), and the determined isothermal bulk modulus and its pressure derivative at 24.6 GPa are K_{TPr} = 110.5(250) GPa and K'_{TPr} = 7.2(25), respectively, with a fixed density of r_{Pr} = 6.43 g/cm^3 at 24.6 GPa. The change in the atomic volume of $Fe_{46.5}Ni_{28.5}S_{25}$ upon melting was found to be ~10% at the melting temperature, a significantly larger value than that of pure Fe (~3%). Combined with the above EoS parameters and the thermal dependence reported in the literature, our data were extrapolated to the outer core conditions of the Earth. Assuming that S is the only light element and considering the range of suggested Ni content, we estimated a 5.3–6.6 wt% S content in the Earth's outer core.

Keywords: Liquid iron alloy, high pressure, Fe_3S, Earth's outer core; Physics and Chemistry of Earth's Deep Mantle and Core