

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

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### ABSTRACT

The density of liquid iron-nickel-sulfur ( $\text{Fe}_{46.5}\text{Ni}_{28.5}\text{S}_{25}$ ) 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  $\text{Fe}_{46.5}\text{Ni}_{28.5}\text{S}_{25}$  at 74 GPa and 3400 K is  $8.03(35) \text{ g/cm}^3$ , 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  $K_{\text{TPr}} = 110.5(250) \text{ GPa}$  and  $K'_{\text{TPr}} = 7.2(25)$ , respectively, with a fixed density of  $r_{\text{Pr}} = 6.43 \text{ g/cm}^3$  at 24.6 GPa. The change in the atomic volume of  $\text{Fe}_{46.5}\text{Ni}_{28.5}\text{S}_{25}$  upon melting was found to be  $\sim 10\%$  at the melting temperature, a significantly larger value than that of pure Fe ( $\sim 3\%$ ). 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,  $\text{Fe}_3\text{S}$ , Earth's outer core; Physics and Chemistry of Earth's Deep Mantle and Core