# Short- and intermediate-range structure and dynamics of Fe-Ni-C liquid under compression

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Properties of liquid Fe alloys under the relevant conditions are crucial for understanding the composition, thermal state, and dynamics of the Earth's core. However, experiments on the liquids are often performed at pressures far below those of the outer core, prompting a long extrapolation of the experimental results to the core condition. Such estimations can be complicated by light elements possibly forming subnormal pressure-dependent molecular clusters that can significantly affect the physical properties as the core condition is approached. The focus of this study is the structural change of Fe-Ni-C liquid with pressure and the role of C in the polyamorphic transition using computation at pressures where experimental results are available. First-principles molecular dynamics was employed to compute properties of the liquid with a composition of $Fe_{3.7}Ni_{0.37}C$ at 1673 K and pressures from 0 to 67 GPa to benchmark the computational methods on the pressure effect on the structure and properties of the liquid at relatively low pressures. The short-range structure is manifested by the coordination number (CN) of the Fe/Ni-Fe/Ni around 12, indicative of a nearly close-packed structure in the pressure range, and the CN of C-Fe/Ni increasing from 6.5 to 8.5, indicative of an approximately octahedral to cubic transition as pressure increases. The Fe/Ni-Fe/Ni bond distance, however, is found to be 10 times more compressed than the C-Fe/Ni. The intermediate-range structure of Fe/Ni-Fe/Ni and C-Fe/Ni subsystems, described by a partial configurationally-decomposed distribution function, undergoes substantial changes, characterized by a significant increase of the number of 3-atom shared polyhedra, which are related to an increased bulk modulus, decreased diffusion coefficient, decreased activation volume for diffusion, and increased shear viscosity. Reproducing the experimental observations at low pressures provides important support to model the liquid under the conditions relevant to the Earth's outer core.

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