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Magnetic and Thermal Fluctuations in Fe and (Fe,Ni) alloys at Earth Core Conditions¹ SUFIAN ALNEMRAT, BORIS KIEFER, New Mexico State University — Several lines of evidence suggest that the earth's inner core is dominated by an iron rich (Fe,Ni) alloy. In this study we address the influence of magnetic and thermal fluctuations as driving forces for phase transitions in Fe and Fe₇Ni structures at inner core pressure and temperature conditions. Bcc iron is stable at ambient conditions due to its ferromagnetic nature which highlights the importance of magnetism for structural stability. *Ab-initio* electronic structure calculations are used to study the thermal and magnetic fluctuations in Fe and (Fe,Ni) alloys up to pressures and temperatures expected in the earth's inner core. The variable cell shape molecular-dynamics simulations include the magnetic moment and thermal fluctuations. Our preliminary results show a phase transformation in hcp-Fe₇Ni alloy that occurs after 2.5 ps, well after equilibration. The correlation of magnetic and thermal fluctuations suggests that the residual magnetism is too weak to induce the observed transition. Instead, large thermal fluctuations at the onset of the transition provide a likely driving force.

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