Abstract Submitted
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Molecular dynamics simulations of equilibrium and undercooled liquid Ni[1] ALVARO POSADA-AMARILLAS, EFRAíN URRUTIA-BAÑUELOS, ROBERTO NÚNEZ-GONZALEZ, Universidad de Sonora, I.L. GARZÓN, Universidad Autonoma de México — Molecular dynamics computer simulations were performed for equilibrium and undercooled liquid Ni. The Gupta potential was used to mimic the interatomic metallic interaction for different thermodynamic states. The inherent structures formalism is used to explore the potential energy landscape, showing a competition between periodic crystalline order (fcc, rhcp and bcc) and regular and distorted icosahedral order. For undercooled liquid Ni, a correlation between the entropy and the change in the crystalline (fcc) and icosahedral order is shown. This is the first simulation study which shows an interplay between the microstructural ordering in undercooled liquid metals and the entropy of the system.

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