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First Principles Study of FCC-HCP Interface Dynamics Under Uniaxial Tension SUNGHO KIM, SEONG-GON KIM, MARK F. HORSTEMEYER, Mississippi State University — We studied the dynamics of FCC-HCP interface of Ni crystal at various tension using first-principles density functional theory(DFT) calculations. Both FCC and HCP structures are closed-packed and different stacking orders. We found that FCC-HCP interfaces can have two different stacking orders. We found that the interface can advance by alternating between two stacking orders under uniaxial tension. Intermediate phases and energy bariers for grain growth of two different phases will be presented.

Seong-Gon Kim
Mississippi State University

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