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First-principles investigation of migration barriers in bulk (Cr,Co)-doped Ni_3Al (γ) and Ni_3Al/Ni (γ'/γ) interface PRIYA GOPAL, SRINIVASAN SRIVILLIPUTHUR, Department of Material Science, University of North Texas — Ni-based super-alloys possess desirable high-temperature properties including ductility, fracture toughness as well as resistance to creep and oxidation mainly due to the precipitation of ordered Ni_3Al γ' precipitates within a γ (Ni,Al) matrix. Various studies have shown that the mechanical properties can be improved by adding substitutional elements. It is thus very important to understand the electronic structure and diffusion kinetics of the substitutional elements and the role each one has on the overall microstructure. \pardthis work we present our results on the systematic study of the energetics and migration barriers of Cr and Co in bulk Ni_3Al and Ni_3Al/Ni (γ'/γ) interface. We did simulations of migration of vacancy and substitutional element in a complete set of migration paths and evaluated the barrier energies in both bulk Ni_3Al and Ni_3Al/Ni (γ'/γ) interface using density functional theory methods. We will briefly discuss our results on the effect of migration barriers on the partitioning behavior of Cr and Co between the and ' phases in Ni-based super-alloy.

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