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Unraveling the Effects of Ta, Re and Mo on Vacancy-mediated Diffusion and Structural Order in γ'-Ni3Al: A Kinetic Monte Carlo Study

Diffusion controls almost microscopic processes such as element partition, microstructure evolution, structural order, and dislocation climb, which is closely related to the creep strength of Ni-based superalloys. In this study, the effects of Re, Mo and Ta on vacancy-mediated diffusion and structural order of γ'-Ni3Al have been systematically evaluated via incorporating first-principles and kinetic Monte Carlo (KMC) simulation. From a thermodynamics perspective, each alloying element increases the barriers of basic diffusion processes of Ni and Al. It is noted that they do not change the preferences diffusion direction of Ni and Al. Specifically, the effects of alloying elements on increasing the inter-sublattice diffusion barriers of Ni and Al follow the sequence of Ta ≈ Re > Mo. For the other basic diffusion processes of Ni and Al, the sequence is Ta > Mo > Re. From a kinetic perspective, KMC simulations indicate that the sequence for reductions in the effects of alloying elements on vacancy diffusion coefficients is Ta > Re > Mo. Each alloying element increases the equilibrium order degree of the γ'-Ni3Al system at high temperatures. It originates from the stable occupations of these alloying elements at Al sublattice sites. Such occupations result in elevated diffusion barriers for Ni migrating to the Al sublattice sites and the decreased equilibrium concentration of NiAl antisite. Further analysis suggests that the structural disorder primarily originates from the limited Ni diffusion processes within inter-sublattice. In contrast, more Al diffusion processes within inter-sublattice contributes less to structural disorder due to their high correlation factor.

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