Strengthening Ni-based superalloys by γ-γ' partitioning regulation of Ta-W/Mo

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ABSTRACT

Ni-based superalloys exhibit complex chemical interactions among various alloying elements, affecting their partitioning behavior between γ-Ni and γ'-Ni_3Al phases. This makes the mechanical properties of superalloys strongly dependent on alloy composition due to the impacts of elemental partitioning on the γ-γ' lattice mismatch and interfacial strength. In this work, the site occupation and partitioning behavior of Ta-X (X=Mo, W) in γ-γ' have been studied by using a novel first-principles method proposed for calculating elemental concentration in co-alloyed dual-phase systems at finite temperature. Our results demonstrate that increasing Ta content suppresses the original substitution tendencies of W and Mo in γ' bulk and leads to their preferential partitioning to γ bulk consequently, thereby reducing the γ-γ' lattice mismatch. Focusing on the γ/γ' interface, W and Mo are verified to segregate on the γ-side layers regardless of Ta's location. Furthermore, the Ta-W/Mo co-alloying is proved to enhance the Griffith work of γ/γ' interface with Ta doped on γ' side. The even stronger strengthening effect of γ'-side Ta-W/Mo co-alloying is attributed to the substitutions of weaker Al-Ni bonds by stronger Ta-Ni, W-Ni and Mo-Ni bonds. This work is expected to provide a theoretical guideline to strengthen the Ni-based superalloys via the regulation of W/Mo partitioning by Ta content.

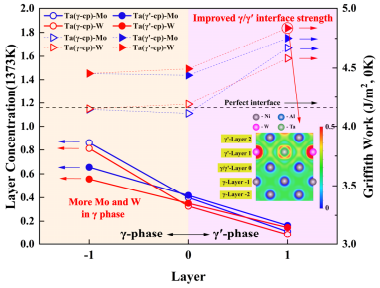

Figure 1: Calculated layer concentrations of alloying atoms X (X=Mo, W) at γ/γ' interface with Ta in γ phase (hollow symbols) and γ' phase (solid symbols) and the corresponding interfacial Griffith works. The electron localization function contour with Ta and W substituting at γ'-corner point (cp) sites is also shown as an inner figure.