Poster Session | F. From Microstructure to Properties: Mechanisms, Microstructure, Manufacturing

[PO-F1]Poster Session 1

Symposium F

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-34]Transition-metal alloying of γ‘-Ni_3Al: Effects on the ideal uniaxial compressive strength from first-principles calculations

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The addition of transition metal (TM) elements into the γ′ precipitate phase of a Ni-based single-crystal superalloy can significantly affect its mechanical properties, including the intrinsic mechanical property of compressive strength. Using first-principles density functional calculations, the effects of 3*d* (Sc-Zn), 4*d* (Y-Cd) and 5*d* (Hf-Au) TM alloying elements on the ideal uniaxial compressive strength of γ′-Ni_3Al were investigated. The stress-strain relationships of pure Ni_3Al under [100], [110] and [111] compressive loads and the site occupancy behavior of TM elements in Ni_3Al were prior studied using a total-energy method based on density functional theory. Our results showed that the capacity of TM elements for strengthening the ideal compressive strength was associated with the *d*-electron number. The alloying elements with half-filled *d*-bands (*i.e.*, Cr, Mo, W, Tc and Re) manifested the greatest efficacy for improving the ideal strength of Ni_3Al under a deformation along the weakest compressive direction. Furthermore, the charge redistribution of Ni_3Al doped with 5*d* elements were also analyzed to understand the strengthening mechanisms of TM elements in the γ′-Ni_3Al phase.