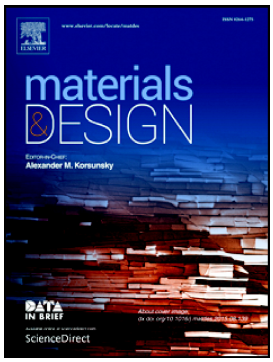
Accepted Manuscript



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PII: S0264-1275(17)30511-7
DOI: doi: 10.1016/j.matdes.2017.05.032
Reference: JMADE 3056

To appear in: *Materials & Design*

Received date: 22 January 2017
Revised date: 21 March 2017
Accepted date: 9 May 2017

Please cite this article as: Shaohua Liu, Minru Wen, Zi Li, Wenqing Liu, Ping Yan, Chongyu Wang , Partitioning and diffusion of transition metal solutes in ternary model Ni-based single crystal superalloys, *Materials & Design* (2017), doi: 10.1016/j.matdes.2017.05.032

Partitioning and diffusion of transition metal solutes in ternary model Ni-based single crystal superalloys

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ABSTRACT

Partitioning and diffusion of transition metal solutes can significantly affect the coarsening rate of γ' precipitates in Ni-based single crystal superalloys. Using first-principles density-functional calculations and atom probe tomography, we investigated the partitioning coefficient and diffusion rate of 3d (Ti–Ni), 4d (Zr–Pd), and 5d (Hf–Pt) transition metal solutes. For ternary model Ni-based single crystal superalloys, the 3d solutes (except Ti) partition to the matrix phase, whereas 4d and 5d solutes (except Ru, Rh, and Ir) prefer γ' precipitates. The existing atom probe tomography results are consistent with the calculation results. Across the periodic table, middle-row elements have a higher (lower) diffusion activation energy (diffusion rate) than early and late row elements. The band-filling effect that is coupled with electronic structure analysis can explain the parabolic behavior of energetics that involve bond breaking. To minimize the coarsening rate, we have screened alloying elements that both have a low diffusion rate in the γ matrix and partition to the γ' phase. These alloying elements will suppress the coarsening behavior of the precipitates and are expected to contribute to the stability of precipitates at elevated temperature.

Keywords: nickel-based superalloy; partitioning coefficient; diffusion rate; coarsening; first-principles; atom probe tomography