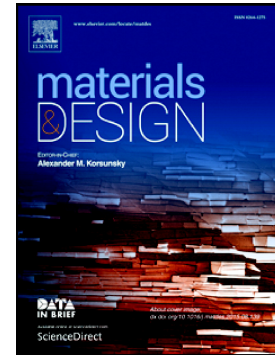


## Accepted Manuscript

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

Shaohua Liu, Minru Wen, Zi Li, Wenqing Liu, Ping Yan, Chongyu Wang



PII: S0264-1275(17)30511-7  
DOI: doi: [10.1016/j.matdes.2017.05.032](https://doi.org/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](https://doi.org/10.1016/j.matdes.2017.05.032)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

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

Shaohua Liu<sup>a</sup>, Minru Wen<sup>b</sup>, Zi Li<sup>c</sup>, Wenqing Liu<sup>d</sup>, Ping Yan<sup>e</sup>, Chongyu Wang<sup>b,e\*</sup>

<sup>a</sup>*School of Materials Science and Engineering, Tsinghua University, Beijing 100084, China*

<sup>b</sup>*Department of Physics, Tsinghua University, Beijing 100084, China*

<sup>c</sup>*Institute of Applied Physics and Computational Mathematics, Beijing 100088, China*

<sup>d</sup>*Key Laboratory for Microstructures, Shanghai University, Shanghai 200444, China*

<sup>e</sup>*Central Iron & Steel Research Institute, Beijing 100081, China*

\*Corresponding author. Address: Department of Physics, Tsinghua University, Beijing 100084, China. Tel.: +86 1062772782. E-mail: cywang@mail.tsinghua.edu.cn (Chongyu Wang).

## ABSTRACT

Partitioning and diffusion of transition metal solutes can significantly affect the coarsening rate of  $\gamma'$  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  $\gamma'$  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  $\gamma$  matrix and partition to the  $\gamma'$  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

Download English Version:

<https://daneshyari.com/en/article/5023160>

Download Persian Version:

<https://daneshyari.com/article/5023160>

[Daneshyari.com](https://daneshyari.com)