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# Influence of composition on microstructural parameters of single crystal nickel-base superalloys

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#### ARTICLE DATA

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#### ABSTRACT

Fourteen nickel-base superalloy single crystals containing a range of chromium (Cr), cobalt (Co), molybdenum (Mo), and rhenium (Re) levels, and fixed amounts of aluminum (Al) and tantalum (Ta), were examined to determine the effect of bulk composition on basic microstructural parameters, including  $\gamma'$  solvus,  $\gamma'$  volume fraction, topologically close-packed (TCP) phases,  $\gamma$  and  $\gamma'$  phase chemistries, and  $\gamma-\gamma'$  lattice mismatch. Regression models describing the influence of bulk alloy composition on each of the microstructural parameters were developed and compared to predictions by a commercially-available software tool that used computational thermodynamics. Co produced the largest change in  $\gamma'$  solvus over the wide compositional range explored and Mo produced the biggest effect on the  $\gamma$  lattice parameter over its range, although Re had a very potent influence on all microstructural parameters investigated. Changing the Cr, Co, Mo, and Re contents in the bulk alloy had an impact on their concentrations in the  $\gamma$  matrix and to a smaller extent in the  $\gamma'$  phase. The software tool under-predicted  $\gamma'$  solvus temperatures and  $\gamma'$  volume fractions, and over-predicted TCP phase volume fractions at 982 °C. However, the statistical regression models provided excellent estimations of the microstructural parameters and demonstrated the usefulness of such formulas.

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#### 1. Introduction

A series of nickel (Ni)-base superalloy single crystals has been developed recently [1–3] in a new compositional design space for potential turbine blade applications. This alloy series, termed LDS (low density single crystal), was explored in an effort to produce single crystal alloys with low densities, while concurrently achieving high temperature creep resistance, microstructural stability, and excellent oxidation resistance. The Ni-base alloy contained fixed contents of aluminum (Al) and tantalum (Ta) for  $\gamma'$  precipitation, as well as variations in the levels of chromium (Cr), cobalt (Co), molybdenum (Mo), and rhenium (Re). Cr was added to the alloy for improved oxidation resistance and was explored [1–3] at relatively low levels to determine minimum Cr concentrations required for sufficient oxidation

resistance. Co was chosen as a conventional superalloy addition, since its density matches that of Ni, and as a result, does not increase alloy density. Co has also been reported to improve alloy stability [4–7]. However, the key alloying strategy employed in this work involved replacing some of the strategic and high density Re, and all of the high density tungsten (W), with Mo for solid solution strengthening. Mo is known to be a potent solid solution strengthener, but has a density almost half that of either Re or W.

The alloys in the present paper represent the compositional design space described above, which is considered novel because of the relatively high Mo content combined with a low Cr level in single crystal form. Superalloy single crystals with high Mo contents were studied earlier [8–10], but these were cast without Cr, Co, and Re, in order to investigate systematically the effects

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of lattice mismatch on  $\gamma'$  coarsening and creep behavior in simple model alloys. Other investigations examined the use of higher Mo contents [11–13], as well as a range of Co [4,5], but these alloys did not contain Re and tended to have higher Cr levels. More recent studies [6,7,14] have examined the effect of Re on various microstructural features. However, these alloys did not contain high Mo contents and included W, ruthenium (Ru), and titanium (Ti) in their compositions along with a number of other significant alloying differences.

The purpose of this paper is to characterize more fully the key microstructural parameters that are known to influence the mechanical properties of nickel-base superalloy single crystals. This paper focuses on the effects of alloy composition on microstructural parameters, including  $\gamma'$  solvus,  $\gamma'$  volume fraction, topologically close-packed (TCP) phase content,  $\gamma$  and  $\gamma'$  phase chemistries, and  $\gamma-\gamma'$  lattice mismatch. In the present study, quantitative assessments of these microstructural features are provided, and regression models are developed to predict these microstructural parameters from bulk alloy composition. Ultimately, these microstructural parameters will be used in the development of a creep model that will be described in a future paper. It is expected that the regression models presented herein, coupled with a creep model, will enable the alloy composition to be fine tuned to obtain microstructural features that deliver targeted mechanical properties. Additionally, the use of computational thermodynamic modeling tools for application to multi-component Ni-base superalloys has become increasingly common. Thus, a commercially-available software package JMatPro 6.0®, an acronym for Java-based Materials Properties software [15,16], was employed to predict the microstructural parameters observed experimentally. It is hoped that the experimental data and its interpretation provided in this paper will also enable improvements in the predictive capability of JMatPro and other computational tools.

### 2. Materials and Experimental Procedures

A design of experiments approach [2,3] was employed that minimized the number of alloys to be cast. Based on this approach, a total of fourteen LDS alloys (Table 1) were cast into

single crystal slabs at a commercial casting vendor, PCC Airfoils LLC, Minerva, OH. The aim baseline alloy selected for this design strategy contained 6.1 wt.% Al, 6.2 wt.% Ta, 50-100 ppm wt. yttrium (Y), and a balance of Ni. Alloying elements were varied as follows: 0-5 wt.% Cr; 0-11 wt.% Co; 6-12 wt.% Mo; and 0-4 wt.% Re. These element ranges were chosen [2,3] to allow for good predictive capabilities within the compositional design space, while enabling attractive alloys for potential applications to be explored. Small quantities of carbon (C) and boron (B) were added as grain boundary strengthening elements, which has been done more recently in third and fourth generation alloys to reduce the impact of undesirable grain boundary defects [2,3] that may be present in turbine blades and to improve superalloy cleanliness [17]. Hafnium (Hf) was added to selected alloys at a nominal level of 0.2 wt.% for oxidation resistance. The slab castings measured approximately 15 cm long in the single crystal growth direction, 5 cm wide, and 0.6 cm thick. The castings were solution treated at a commercial heat treatment vendor; the solution temperature was reached by a series of step increments to avoid incipient melting and overshooting. Single crystal castings without Hf additions were solution treated for 6 h at 1315 °C, and castings with Hf were solution treated for 6 h at 1305 °C. Because of its lower solidus, LDS-1110 was given a step heat treatment with a solution temperature of 1288 °C for 18 h at Glenn Research Center. All castings were fan quenched in argon from the solution temperature to temperatures below 1093 °C at a rate of 43 °C/min.

Bulk chemical analyses were performed by inductively coupled plasma emission spectroscopy (ICP) at the top and bottom sections of at least one casting of each composition. In addition, trace impurity levels of sulfur (S) were analyzed in selected alloys by Glow-Discharge Mass Spectroscopy (GDMS) at SHIVA Technologies, Syracuse, New York. Pins, nominally 1.6 mm square by 19 mm long, were supplied for this latter analysis.

Differential Thermal Analysis (DTA) was conducted on LDS alloys in a helium atmosphere using a Netzsch STA 409C instrument. Selected alloys were examined in the as-cast condition, and all alloys were analyzed in the as-solutioned condition. The 1500 mg single crystal samples were heated at a rate of 10  $^{\circ}$ C/min in a high purity alumina crucible from 20  $^{\circ}$ C

Table 1 – Analyzed Compositions (wt.%) of Single Crystal Alloys.													
Alloy	Cr	Co	Мо	Re	Al	Ta	Hf	Y	Ni	В	С	S (ppm wt.)	
LDS-0010	0.00	0.00	12.02	0.00	6.08	6.14	0.00	0.0053 top 0.0277 bottom	75.6	0.0040	0.0140	n/a <sup>a</sup>	
LDS-0101	0.01	9.76	7.01	2.92	6.01	6.28	0.00	0.0070 top 0.0180 bottom	67.9	0.0045	0.0098	n/a <sup>a</sup>	
LDS-5051	2.35	0.00	9.01	2.99	6.03	6.11	0.00	0.0065 top 0.0174 bottom	73.4	0.0040	0.0140	2.8	
LDS-5555	2.43	4.91	9.48	1.48	6.03	6.17	0.00	0.0046 top 0.0187 bottom	69.4	0.0032	0.0168	2.8	
LDS-4583	3.90	5.00	8.10	3.00	6.00	6.30	0.20	0.0057 top 0.0067 bottom	67.3	0.0030	0.0104	2.8	
LDS-4183	3.93	9.97	8.13	3.04	6.05	6.22	0.20	0.0073 top 0.0069 bottom	62.4	0.0030	0.0139	3.2	
LDS-4164	4.00	11.00	6.10	4.10	6.00	6.20	0.20	0.0073 top 0.0114 bottom	62.4	0.0040	0.0110	n/a <sup>a</sup>	
LDS-1000	4.79	0.00	7.08	0.00	6.04	6.21	0.00	0.0048 top 0.0210 bottom	75.8	0.0030	0.0098	3.1	
LDS-1501	4.93	4.98	7.13	3.05	6.01	6.26	0.19	0.0057 top 0.0118 bottom	67.4	0.0030	0.0098	n/a <sup>a</sup>	
LDS-1101	4.70	9.90	7.10	3.00	6.00	6.20	0.00	0.0050 top 0.0193 bottom	63.1	0.0035	0.0160	4.1	
LDS-1164	4.90	10.00	6.10	4.00	6.00	6.30	0.20	0.0042 top 0.0084 bottom	62.5	0.0030	0.0130	n/a <sup>a</sup>	
LDS-1101+Hf	5.00	10.00	7.30	3.10	6.10	6.50	0.19	0.0079 top 0.0076 bottom	61.7	n/a	0.0240	0.87	
LDS-1182	4.88	9.99	8.19	2.03	5.99	6.25	0.22	0.0066 top 0.0044 bottom	62.4	0.0040	0.0097	n/a <sup>a</sup>	
LDS-1110	4.68	9.76	11.95	0.00	5.98	6.08	0.00	0.0047 top 0.0177 bottom	61.4	0.0030	0.0180	n/a <sup>a</sup>	
a n/a=not mea	a n/a=not measured.												

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