Designing a Recrystallization Kinetics Model for Dilute Niobium Alloys

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Introduction

The refractory metals (W, Ta, Nb, Re, Mo) perform particularly well in extreme environments due to their high strength and resistance to heat. Niobium has a low density relative to the other refractories and other materials with comparably desirable properties, therefore it is a popular choice for the base element of aerospace alloys[1] (e.g. C103, WC3009, CB752). While it is known that alloying Nb with elements such as Ti, Hf, and Zr can yield desirable macro-scale properties, little has been studied about why and how these alloying elements work on an atomic level to change niobium's performance from a microstructural perspective.

Basis of Study – 3 Nb Alloys

Table I: *Estimated RX Temperatures for alloys*

Alloy (99 at% Nb)	RX Temp (°C)
1 at% Ti	~ 700
1 at% Hf	~ 1100
1 at% Zr	~ 1400

Objective: build a theory for why difference in behavior occurs in two project phases:

1) **Initial Modeling:** Build Models of predicting X_V as a function of t and T for each alloy
2) **Master Modeling:** Use the initial models to build a new model predicting X_V as a function of solute atom properties (size, bond lengths, melting T, etc.)

Experimental Methods

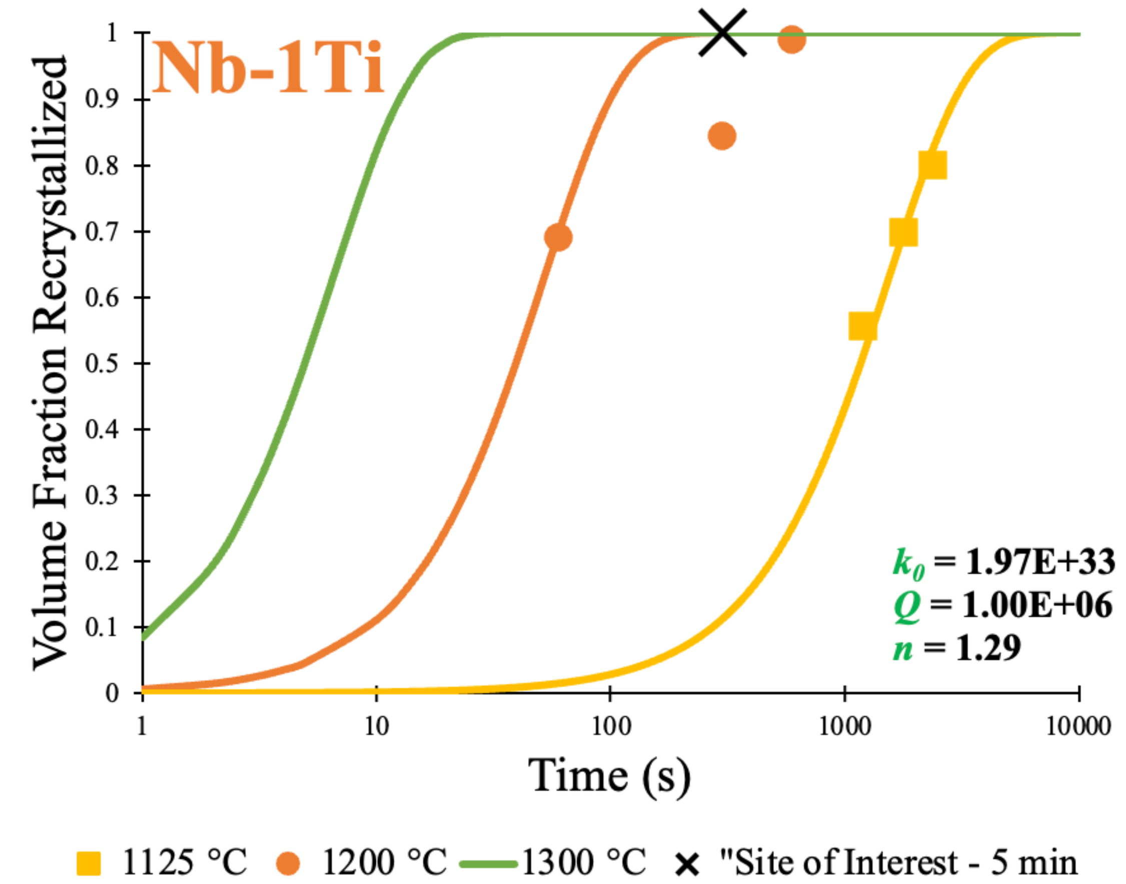
- Melt Alloys → Cold-Roll to 90% Reduction → Cut 10 mm Width Samples
- Encapsulate in Quartz Tubes → Seal Tubes Under Vacuum → Anneal / Quench
- Mount / Polish → Image Using SEM BSE / EBSD → Analyze for X_V Using ASTM E562

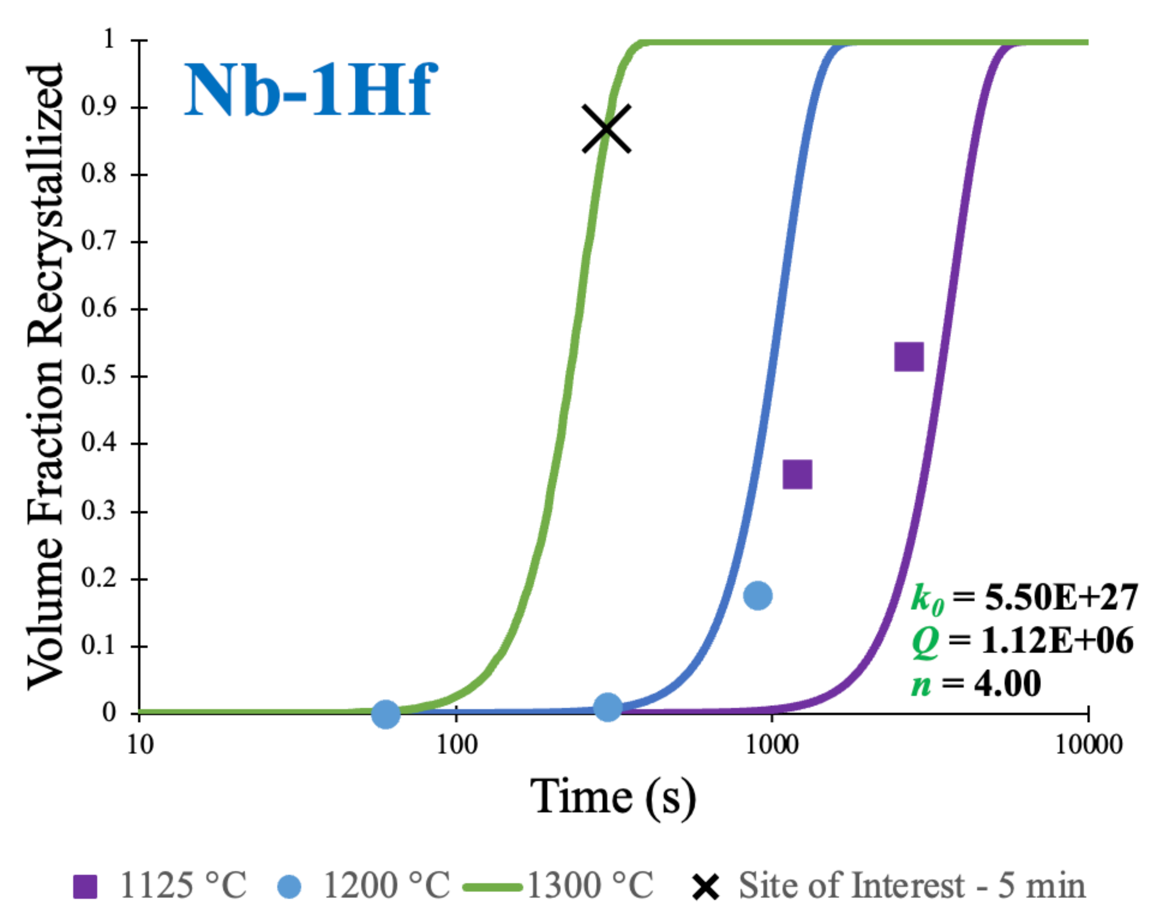
Results – Initial Models

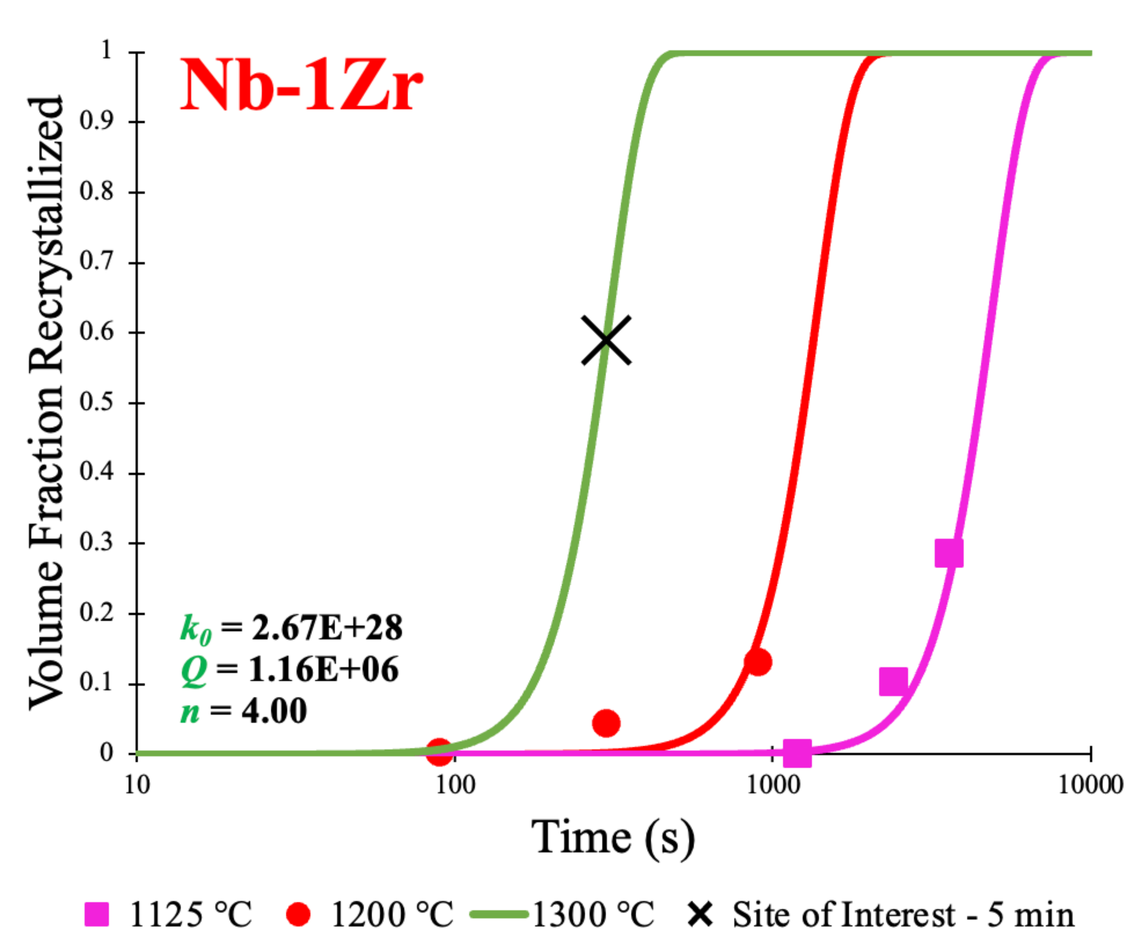
1) Initial Modeling: The models below were built using least squares polynomial fit to **Equation 1** with variables k_0, Q, and n, as fit parameters. The green curves show each model's prediction for RX behavior at 1300 °C.

JMAK Theory Used for Model Building[2]

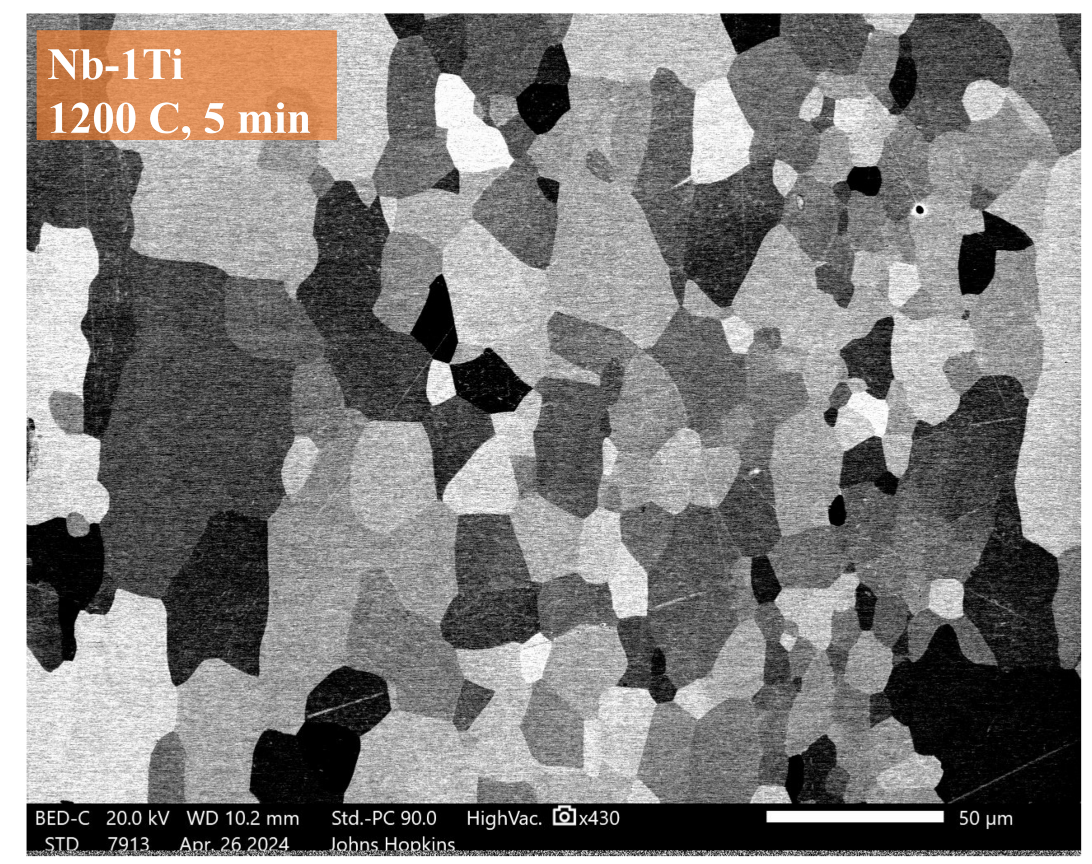
$$X_V = 1 - \exp(-kt^n), \text{ where } k = k_0 \exp\left(-\frac{Q}{RT}\right) \quad (1)$$



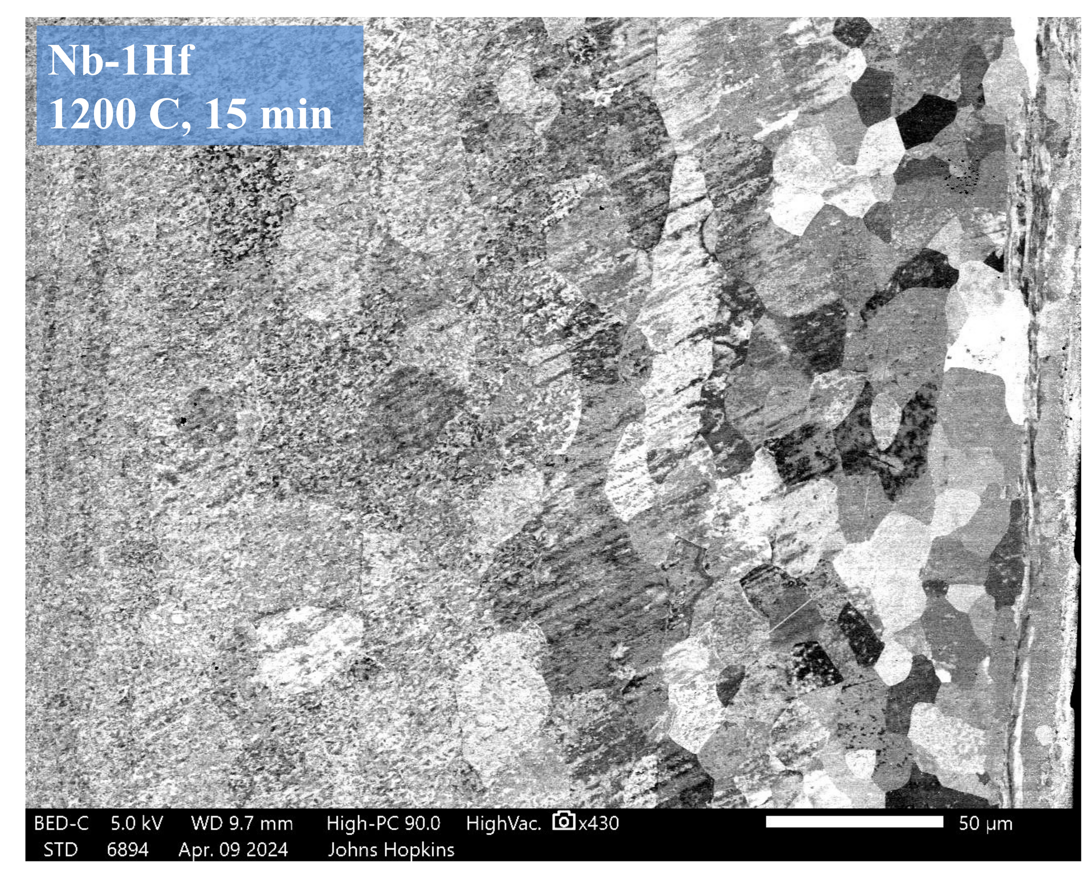




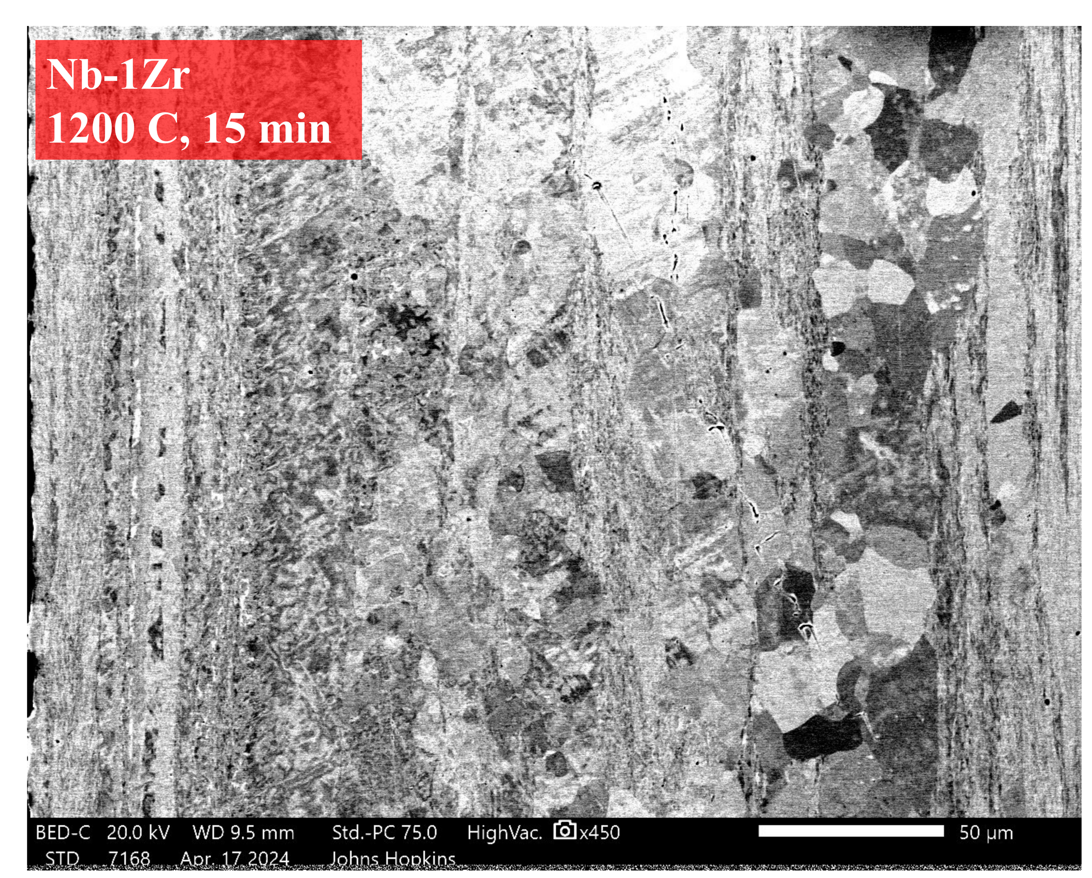
Comparison of Microstructure at Similar Processing Conditions



After 5 min at 1200 °C, Nb-1Ti is fully recrystallized and grain growth occurs



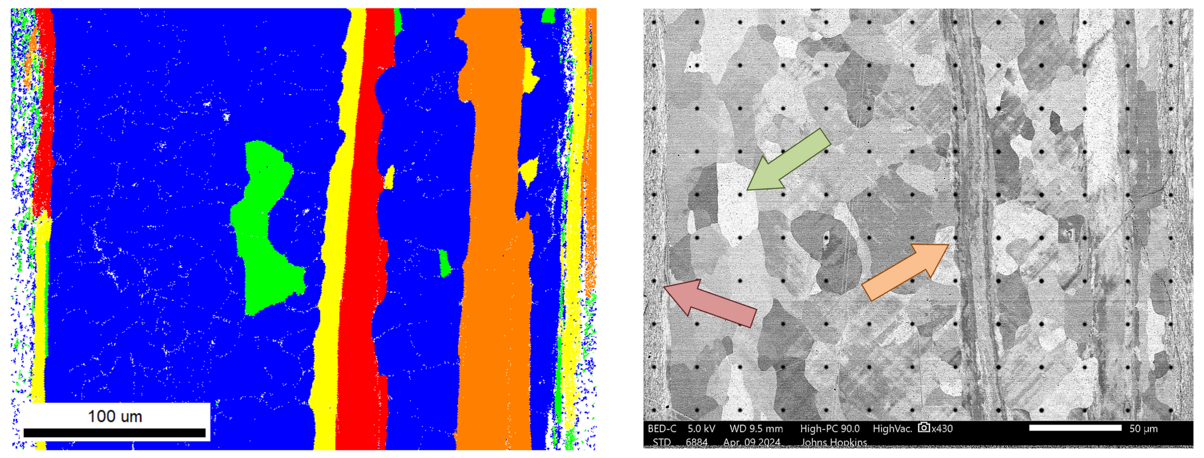
After 15 min at 1200 °C, Nb-1Hf is 17.7% recrystallized



After 15 min at 1200 °C, Nb-1Hf is 13.2% recrystallized

Analysis

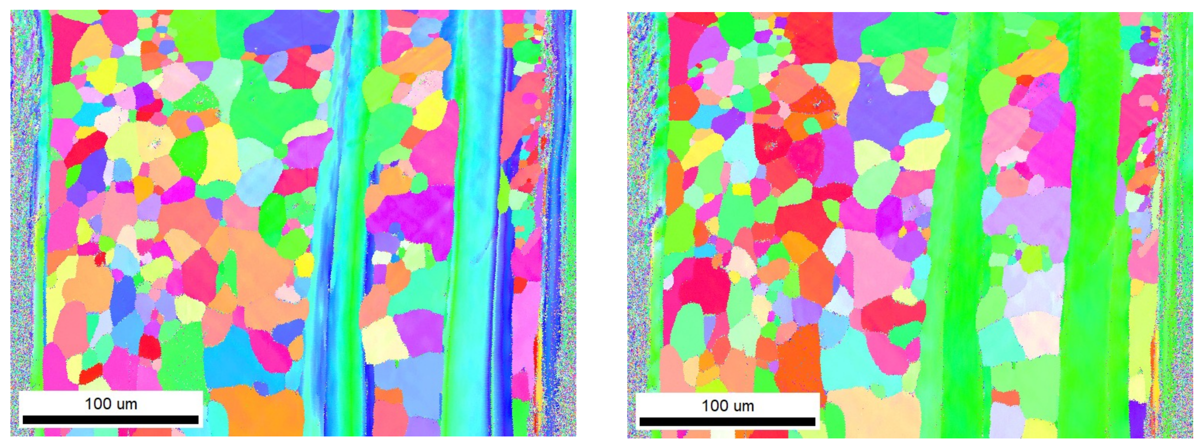
The accuracy of the ASTM E562 method was confirmed using EBSD analysis on one sample. For Nb-1Hf after 45 min at 1125 °C , grain orientation mapping measured 64.4% RX and ASTM E652 measured 63.1% RX.



Color Coded Map Type: Grain Orientation Spread

	Min	Max	Total Fraction	Partition Fraction
Blue	0	2	0.644	0.644
Green	2	4	0.041	0.041
Yellow	4	6	0.068	0.068
Orange	6	8	0.117	0.117
Red	8	15	0.070	0.070

$$\frac{75 + 14 + 41}{130} = X_V$$



EBSD grain orientation scans of Nb-1Hf after 45 min at 1125 °C in rolling direction (left) and transverse planes (right)

Future Directions

Phase 1, initial modeling, is nearing the end of completion. As shown in the plots to the left, there is a lack of data populating the "linear" region of the sigmoidal JMAK curves. Before moving into **Phase 2, master modeling,** I plan to complete additional annealing trials at 1125 and 1200 °C and initial trials at 1050 °C to populate the datasets and reduce the uncertainty of the base models.

References & Acknowledgements

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[1] Satya Prasad, V.V., Baligidad, R.G., Gokhale, A.A. (2017). Niobium and Other High Temperature Refractory Metals for Aerospace Applications. In: Prasad, N., Wanhill, R. (eds) Aerospace Materials and Material Technologies . Indian Institute of Metals Series. Springer, Singapore. https://doi.org/10.1007/978-981-10-2134-3_12

[2] Kalu, Peter & Waryoba, Daudi. (2007). A JMAK-microhardness model for quantifying the kinetics of restoration mechanisms in inhomogeneous microstructure. Materials Science and Engineering A. 464. 68-75. 10.1016/j.msea.2007.01.124.