

Bayesian Analysis of Grain Size Across Variants of α-HCP Crystal Laths in Additively Manufactured Ti-6Al-4V



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Bayesian Statistics

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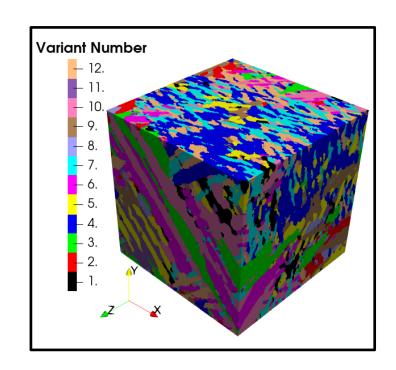
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MOTIVATION



- Plastic deformation in metals can only happen in specific directions (slip systems);
- LPBF Ti64 is composed of a collection of parent
 β-BCC grains, each one leading to up to 12 unique
 α-HCP crystal variants with distinct crystallographic and morphological orientations;
- HCP crystals are highly anisotropic.



GRAIN SIZE DIRECTLY AFFECTS THE OVERALL MATERIAL BEHAVIOR!



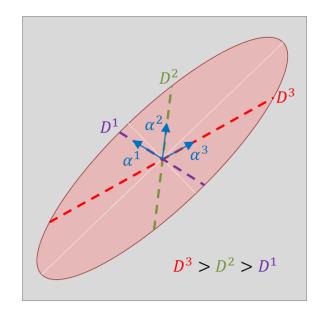
PRELIMINARY LITERATURE REVIEW



• Hall (1951)¹ and Petch (1953)² described what is now known as Hall-Petch effect, or grain boundary strengthening:

$$g_{HP}^{\alpha} \propto \frac{1}{\sqrt{D^{\alpha}}}$$

- Nye (1953)³ introduced the concept of GNDs to accommodate strain gradients across grains.
- Zhao et al (2018)⁴ summarizes the most common morphological orientations of laths of each variant.



• In the field review by Bartolomeu et al $(2022)^5$, they indicate the most common approach as treating the α phase as a whole.

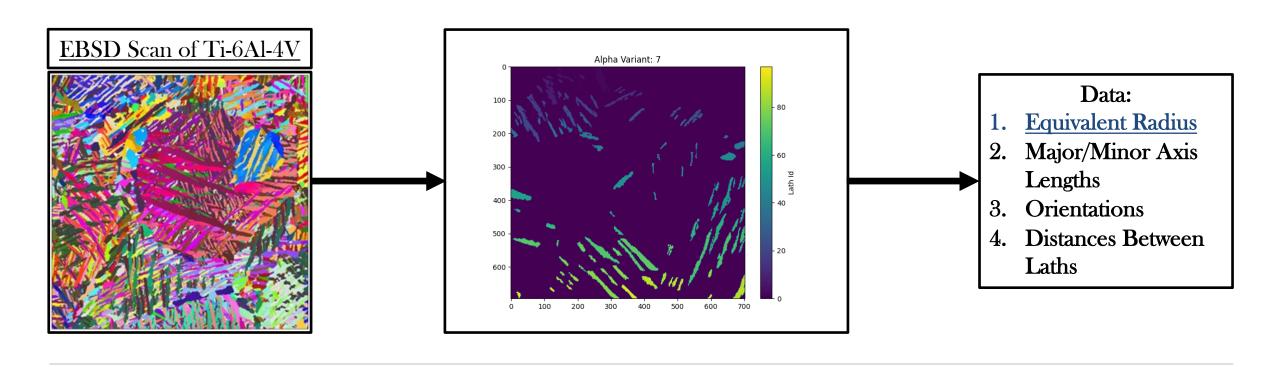
WE PLAN ON ACCOUNTING FOR EACH VARIANT INDEPENDENTLY!



SOURCE OF DATA



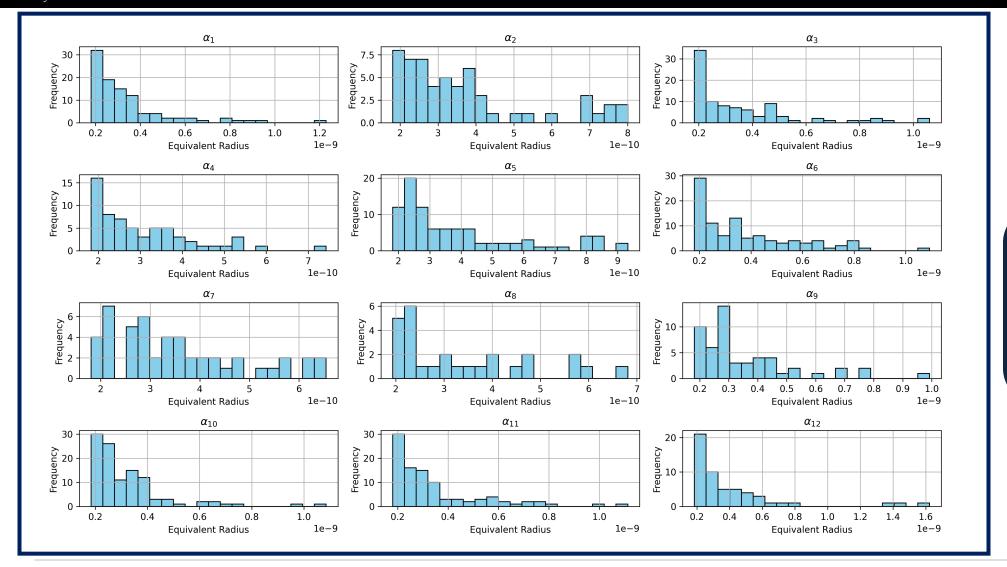
- Electron Backscatter Diffraction (EBSD) scans of Ti-6Al-4V;
- Filter noise from the experiment;
- Identify α -HCP crystal laths, their variants, and record data.





RELEVANT DESCRIPTIVE STATISTICS



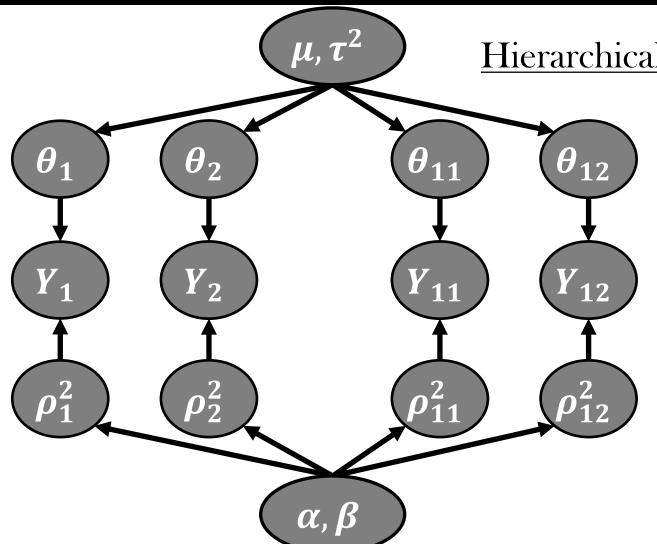


WHAT IS THE
RELATIONSHIP
BETWEEN
VARIANT AND
LATH SIZE?



METHODS FOR BAYESIAN ANALYSIS





- Hierarchical Model with Non-Constant Variance
 - Hierarchical model for both means and variances
 - Model allows for the possibility of the population variances to vary across groups

Distributions:

- 1. $Y_i \sim LogNormal$
- 2. $\theta_i \sim Normal$
 - 1. μ ~Normal
 - 2. $\tau^2 \sim Gamma$
- 3. $\rho_i^2 \sim Gamma$
 - 1. $\alpha \sim Geometric$
 - 2. β~Gamma

Priors:

- 1. $\mu \sim Normal(9.9, 10)$
- 2. $\tau^2 \sim Gamma(1, 0.05)$
- 3. $\alpha \sim Geometric(1)$
- 4. $\beta \sim Gamma(1, 100)$

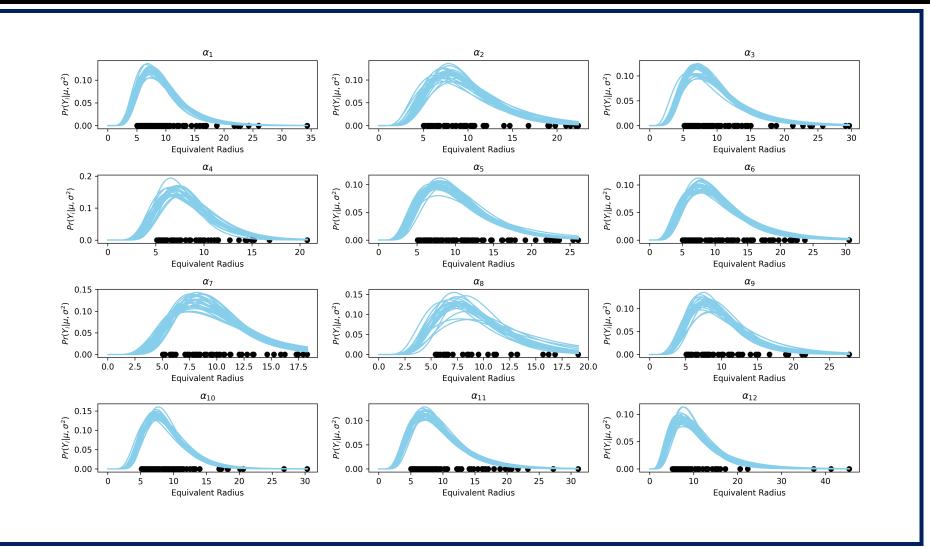


PRELIMINARY FINDINGS



Plots of Sampling Model

- These plots show the sampling model using the final 20 samples from the Gibbs Sampler
- Plots are displayed for each α variant



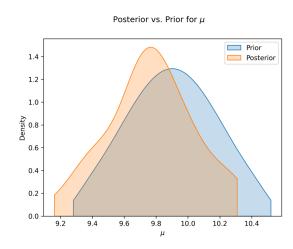


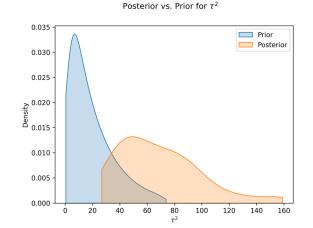
PRELIMINARY FINDINGS

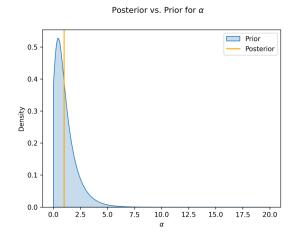


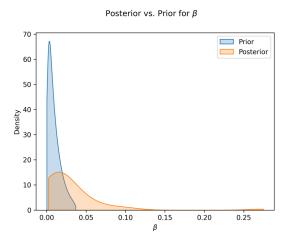
Prior vs. Posterior Plots for Between Group Variables

- These plots show the difference in the prior distributions and the posterior distributions (conditioned on data)
- Many of the prior distributions appear to not resemble the posterior distributions
- Problematic results relating to the estimation of the posterior for α











CONCLUDING REMARKS



- Work here represents the simplified case of estimating only the equivalent radius
- Further research needs to be done pertaining to the α term
- Significantly more information can be earned by using a multivariate distribution for the major and minor axis
- Further information can be earned through inferring the probability of the distance between lath given the sizes of the laths
 - Will need to be a regression model





FINAL SLIDE



REFERENCES



- 1. Hall, E.O. (1951). "The Deformation and Ageing of Mild Steel: III Discussion of Results". *Proc. Phys. Soc. Lond.* **64** (9): 747–753.
- 2. Petch, N.J. (1953). "The Cleavage Strength of Polycrystals". *J. Iron Steel Inst. London*. **173**: 25–28.
- 3. Nye, J.F (1953). "Some geometrical relations in dislocated crystals". *Acta Metallurgica*. **1** (2): 153–162.
- 4. Zhao, Z. B., Wang, Q. J., Wang, H., Liu, J. R. & Yang, R. (2018). "Determining the orientation of parent β grain from one α variant in titanium alloys". *J. Appl. Cryst.* **51**: 1125-1132.
- 5. Bartolomeu, F., Gasik, M., Silva, F.S., Miranda, G. (2022). "Mechanical Properties of Ti6Al4V Fabricated by Laser Powder Bed Fusion: A Review Focused on the Processing and Microstructural Parameters Influence on the Final Properties". *Metals.* **12**: 986.