

**Bayesian Inference Approach to Estimating Elastic Constants of β
Metastable Titanium Alloys Using High-Energy X-ray Diffraction and
Micromechanical Modeling**

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Bayesian Inference

*High-Energy X-ray
Diffraction (HE-XRD)*

Elastic Constants

Abstract

In this study, we present an approach using Bayesian inference framework to estimate single-crystal elastic constants (SEC) in two-phase near- β titanium alloy (Ti-10V-2Fe-3Al, or Ti-1023). This methodology integrates high-energy X-ray diffraction (HE-XRD) data from the Diamond synchrotron source with elastic self-consistent (ELSC) micromechanical modeling [1] to analyze lattice strains across various grain orientations during in situ loading

HE-XRD provides insights into the elastic anisotropy via characterization of lattice strains across different grain orientations under loading. Meanwhile, the ELSC model aids in simulating the mechanical behavior of polycrystalline aggregates to understand the grain-scale deformations.

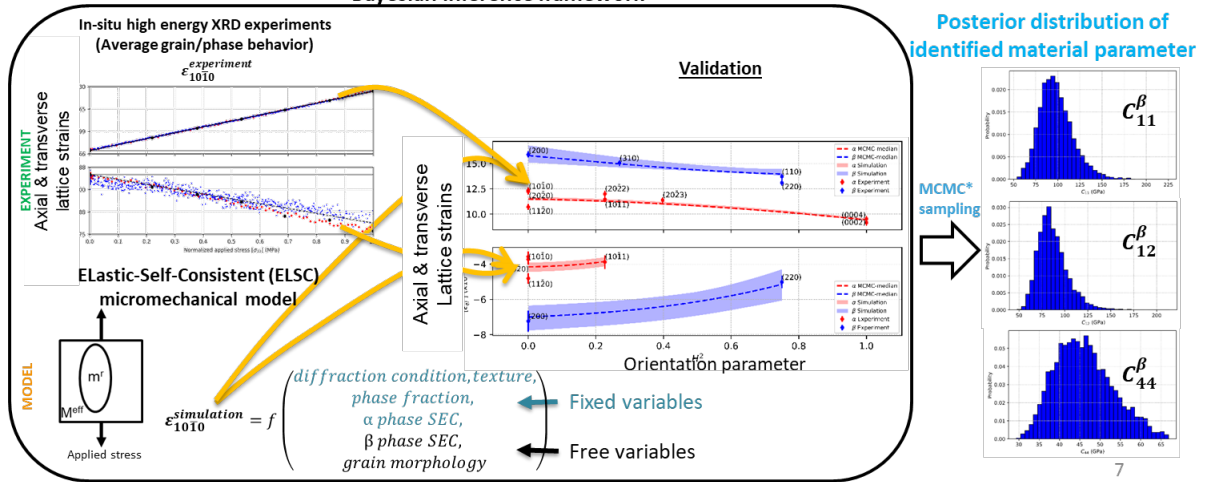
The talk will illustrate how Bayesian inference framework (Figure 1) can be effectively used to address uncertainties and provide statistical estimates of SEC [2]. We have systematically investigated the effect of different material parameters (crystallographic and morphological textures, phase volume fraction) of the micromechanical model and the biases introduced by the XRD data on the identification of the SEC of the β phase. Our study highlights the role of grain morphology on the SEC estimation - often oversimplified in literature.

Bayes theorem:

$$P(\theta|x) = \frac{P(x|\theta) P(\theta)}{P(x)}$$

θ → model parameters to be identified
 x → Exp. Data to evaluate the model
 $P(x|\theta)$ → Likelihood function;
 $P(\theta)$ → Prior belief
 $P(\theta|x)$ → Posterior belief

Bayesian inference framework*



*MCMC: Markov Chain Monte Carlo

Figure 1 – Markov Chain Monte Carlo framework for estimation of single crystal elastic constants distribution

References

- [1] C. Mareau, S. Berbenni, An affine formulation for the self-consistent modeling of elasto-viscoplastic heterogeneous materials based on the translated field method, *Int. J. Plast.* 64 (2015) 134–150.
- [2] R.R.P. Purushottam Raj Purohit, T. Richeton, S. Berbenni, L. Germain, N. Gey, T. Connolley, O. Castelnau, Estimating single-crystal elastic constants of polycrystalline β metastable titanium alloy: A Bayesian inference analysis based on high energy X-ray diffraction and micromechanical modeling, *Acta Materialia*. 208 (2021).