Nondestructive quantification of single crystal elasticity for additively manufactured SB-CoNi-10C, IN625, and Ti64

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Abstract

Resonant ultrasound spectroscopy (RUS) is capable of determining the single crystal elastic constants from polycrystalline specimens with known crystallographic texture. However, the calculated single crystal elastic constants vary with the measured texture, resulting in inconsistent estimates for additively manufactured (AM) specimens with heterogenous texture regions. In this work, the accuracy of the determined single crystal elastic constants is improved by incorporating the uncertainty of the texture in the determination of single crystal elasticity, and requiring only small quantities of electron backscatter diffraction data (EBSD) to do so. The single crystal elastic constants are determined by Bayesian inference with parallelized sequential Monte Carlo (SMC), enabling an order of magnitude reduction in computational cost. AM specimens of a cobalt-nickel-base superalloy (SB-CoNi-10C) demonstrate that the incorporation of texture variability enables the single crystal elastic constants to converge to the reported literature values within one standard deviation, avoiding any dependence on the initial texture values. The single crystal elastic constants of nickel-base-superalloy Inconel 625 (IN625) and Ti-6Al-4V (Ti64) are determined from AM specimens, using only RUS and EBSD data. The determined single crystal elastic constants of IN625 agree between two different texture conditions (induced by AM raster strategy), as well as with the literature values, within one standard deviation. The single crystal elastic constants determined from three AM Ti64 specimens, printed with different beam powers, agree with the range of literature values within two standard deviations but demonstrate variability between AM specimens, indicating that the frequencies may be susceptible to the effects of secondary phases.

1 Introduction

Single crystal elastic constants describe the fundamental mechanical response of crystalline materials. Knowledge of the single crystal elastic constants is critical for property prediction of materials with variable microstructures, such as additively manufactured (AM) components. Recent work [1] has shown that even with a constant set of processing parameters, part groupings of various sizes can inadvertently lead to significant variations in crystallographic texture and mechanical properties. Despite the importance of accurate knowledge of the single crystal elastic constants, historical measurements required the growth of a single crystal specimen and mechanical [2, 3] or ultrasonic [4, 5, 6] testing. Though calculations based on Density Functional Theory (DFT) have risen to quantify the single crystal elastic constants [7], experimental measurements are capable of higher precision and serve as critical validation. Because single crystal growth requires high cost equipment and expertise, there is a driving force for the determination of the single crystal elastic properties from polycrystalline specimens [8, 9, 10]. Unfortunately, the majority of the polycrystal-based approaches still require access to synchrotron facilities.

Consequently, techniques to quantify the single crystalline elastic properties from polycrystals on the laboratory scale are of interest. Recently, ultrasound has been used to determine the single crystal elastic constants from bulk elastic properties of polycrystalline materials [11, 12]. These efforts involve the use of localized surface acoustic wave measurements [11] or bulk ultrasound measurements [12] to infer the single crystal properties. Given the low expense of these ultrasonic approaches, the authors of this work have previously developed a method [13] to inversely determine the single crystal elastic constants from resonant ultrasound spectroscopy (RUS) measurements of (textured) additively manufactured specimens. Critically, this work incorporates Bayesian inference into the inverse determination of the single crystal elastic constants, generating probability distributions and uncertainties on each independently determined parameter, directly from the measured resonant frequencies. However, the previous work by the authors [13] required the specimen's crystallographic texture (preferential crystallographic orientation of grains) as a fixed input to the calculation, resulting in the single crystal elastic constants depending on both the method and quantity of texture data collected.

This research serves to increase the accuracy and consequent reliability of the single crystal elastic constants as determined from RUS measurements on AM specimens, by incorporating uncertainty in the supplied texture as determined by electron backscatter diffraction (EBSD) measurements. The research presented here further develops the Bayesian inference framework created by the authors in [13], and is demonstrated to increase the accuracy of the single crystal elastic constants when determined from AM specimens. Cobalt-nickel-based superalloy (SB-CoNi-10C) specimens and texture data, originally studied in [13], are re-examined to demonstrate the improvements in the determined single crystal elastic constants. The novel framework is then used to quantify the single crystal elastic constants of AM Inconel 625 (IN625) and AM Ti-6Al-4V (Ti64) using only the resonant frequencies and EBSD data.

The novelty of this work is: 1. The development of a framework to determine the single crystal elastic constants from RUS measurements, incorporating texture uncertainty for both cubic and hexagonal materials. 2. To calculate textural uncertainty from EBSD data, in order to increase the accuracy of the determined single crystal elastic constants from RUS data without extensive texture measurements. 3. The demonstration of more accurately determined single crystal elastic constants, independent of the initial texture data, by studying a SB-CoNi-10C AM specimen characterized with both neutron diffraction [13] and EBSD. 4. To report the single-crystal elastic constants of IN625 and Ti64 from AM specimens, and compare with reported literature values.

The paper is organized in the following sequence: The printing parameters of each AM build are detailed in Section 2. The computations to determine the single crystal elastic constants from the resonant frequencies are described in Section 3. The determination of texture variability within each EBSD dataset for input to the inverse model is described in Section 3.1. The independent parameters involved in the inverse calculation of the single crystal elastic constants of each printed AM material, along with the construction of the forward model to calculate resonant frequencies from the single crystal elastic constants, are described in Section 3.2. The inverse solving of the single crystal elastic

constants with sequential Monte Carlo (SMC) is described in Section 3.3. The estimated single crystal elastic constants of SB-CoNi-10C, IN625, and Ti64 are provided in Section 4 and compared to the single crystal elastic constants reported in the literature. The dependencies of the resultant single crystal elastic constants on AM processing conditions are discussed.

2 Materials and methods

2.1 SB-CoNi-10C: Laser powder bed fusion

An Aconity3D AconityMINI¹ system at the University of California Santa Barbara was used to print rectangular SB-CoNi- $10C^2$ specimens with nominal dimensions of 10 mm x 10 mm x 13 mm, with the build direction (BD) parallel to the 13 mm dimension. Virgin powder was used, with printing details reproduced from [13, 14]. The powder was provided by Carpenter Technologies³, with composition given in Table 1.

SB-CoNi-10C Chemical analysis (% mass fraction)										
	Co	Ni	Al	W	Ta	Cr	С	В	Y	Hf
Powder	Bal.	35.93	5.98	3.06	10.40	5.24	0.069	0.013	0.006	0.057

Table 1: Chemical analysis of SB-CoNi-10C powder prior to build as measured by Carpenter Technologies. Major constituents were measured by X-ray. B was measured by mass spectrometry and Y was measured by wet-chem analysis. Quantities in % mass fraction.

A bi-directional scan strategy with a 90° rotation between build layers was utilized with the build plate preheated to 200°C. The beam power was 130 W, the scan speed was 0.833 m/s, the beam diameter was 80 μ m, and the layer thickness was 30 μ m. As described in [14], wire electrical discharge machining (EDM) was used to remove ~0.75 mm of material from each of the six surfaces of the as-printed SB-CoNi-10C rectangular parallelepiped. An additional ~1 mm of material was removed from the side of the asprinted specimen that was connected to the build plate. The specimen was polished with 600-grit sandpaper to a final geometry of 10.355 mm x 8.883 mm x 8.370 mm, with a measured density of 8594 $\frac{kg}{m^3}$. A ±1% dimensional tolerance was considered the maximum allowable uncertainty during specimen preparation, correlating to $\leq \pm 25 \ \mu$ m following measurement with a set of vernier calipers. A stress relief heat treatment at 1100°C for 2h was performed after sectioning and polishing, with measurements of the specimen dimensions showing no difference after heat treatment, considering the $\pm 25 \ \mu$ m precision.

Texture data of the specimen was gathered and reported in [13] by both EBSD and neutron diffraction. EBSD data was gathered across a $\sim 3.5 \text{ mm x } 9.0 \text{ mm}$ area of the sectioned specimen face. To reduce distortion, individual 2.0 mm x 3.0 mm scans were performed and then aggregated using the MATLAB toolbox, MTEX¹ [16, 17]. An FEI Versa 3D Dualbeam microscope with an EDAX OIM-Hikary XM4 detector was used for all EBSD scans. All EBSD data was gathered using a scanning electron microscope (SEM) accelerating voltage of 30 kV and current of 6.4 nA. Raw EBSD pattern images were collected for indexing with the EMSphInxEBSD package [15]. Points below a confidence

¹Commercial equipment, instruments, or materials are identified only in order to adequately specify certain procedures. In no case does such identification imply recommendation or endorsement by the US Government, National Institute of Standards and Technology, or NASA, nor does it imply that the products identified are necessarily the best available for the purpose.

²Commercially available at Carpenter Technologies³ as Gamma Print 700

 $^{^{3}\}mathrm{Carpenter}$ Technology, 1735 Market Street, 15th Floor, Philadelphia, PA 19103 USA



Figure 1: Sectioning strategy (black dashes) of the as-built block, approximate EBSD measurement area (blue dashes), and EBSD data for the SB-CoNi-10C specimen. EBSD data was gathered as individual overlapping scans. Inverse pole figure coloration is referenced relative to the build direction (BD). EBSD pattern indexing was completed using the EMSphInxEBSD package [15].

index of 0.18 (<10% of the datapoints) were removed prior to orientation distribution function (ODF) generation in MTEX. The EMSphInxEBSD-indexed scans are shown in Figure 1.

Neutron diffraction measurements, carried out at Los Alamos National Laboratory with the high-pressure preferred orientation (HIPPO) diffractometer [18, 19], are reproduced from [13]. The Rietveld refinement software, Material Analysis using Diffraction (MAUD) [20], was used to analyze the neutron diffraction data following the procedure of [21]. In brief, the software fits a diffraction spectra to the measured spectra via iterative minimization of least squared error. Consistent with [21, 22], the "R"-values intrinsic to the refinement process were examined after each successive refinement to determine the data fit. The weighted (R_{wp}) R-values are given in this work [21, 22], where lower R-values generally indicate better peak fits. After four refinements, the specimen had an R-value of 6.8%. An alternate refinement (referred to as non-convergent) with artificially sharpened texture, resulting in R = 13.2%, was used to examine the influence of the texture analysis on the single crystal elastic constants.

2.2 Inconel 625: Laser powder bed fusion

IN625 Chemical analysis (% mass fraction)																
	Ni	Cr	Fe	Mo	Nb	Co	Ti	Al	Si	Mn	Р	Ta	C	S	0	Ν
Powder	Bal.	20.86	0.62	9.03	3.95	0.17	0.35	0.31	0.07	0.04	< 0.010	< 0.01	0.01	< 0.005	0.022	0.008
Solid	Bal.	20.00	0.80	8.80	3.80	-	0.37	0.32	0.10	0.05	0.006	-	0.01	< 0.001	-	0.0001

Table 2: IN625 composition of powder and solid measured by inductively-coupled plasma atomic emission spectroscopy for all elements (ASTM E1479) except C/S measured by combustion (ASTM E1019) and O/N measured by fusion (ASTM 1019) [23]. All measurements are in % mass fraction.

Inconel 625 (IN625) specimens were provided by the National Institute of Standards

and Technology (NIST) corresponding to the AM Bench 2022-04 modeling challenge⁴ [23]. Specimens were printed by laser powder bed fusion (LPBF) with an EOS $M270^{1}$ in two different raster conditions, 'X' corresponding to a 180° scanning direction rotation between build layers and 'XY' corresponding to a 90° rotation between build layers. The laser power was 195 W, scan speed 800 mm/s, hatch spacing 100 μ m, and layer thickness $20 \ \mu m$. Virgin powder was used for the build. Rectangular specimens were printed with nominal dimensions of ~ 15 mm (x, raster direction) x 10 mm (y) x 20 mm (z, build direction). One printed specimen of each raster condition (X, XY) was chosen for further study, with two rectangular parallelepiped specimens sectioned with EDM from each selected specimen to nominal dimensions 6.5 mm (x, raster direction) x 8.5 mm(y) x 11.0 mm (z, build direction). A $\pm 1\%$ dimensional tolerance was considered the maximum allowable uncertainty during specimen preparation, correlating to $\leq \pm 25 \ \mu m$ following measurement with a set of vernier calipers. The sectioning strategy is shown in Figure 2. Each specimen was sectioned ~ 3 mm from the build plate to avoid epitaxially affected grain growth, with a minimum of 0.5 mm 'skimming' cuts along each specimen surface to remove near-surface grain regions. The four total specimens are denoted X_S1, X_S2, XY_S1, XY_S2 with measured densities 8415 $\frac{kg}{m^3}$, 8410. $\frac{kg}{m^3}$, 8429 $\frac{kg}{m^3}$, and 8412 $\frac{kg}{m^3}$, respectively.

The EBSD scans were gathered by NIST on duplicate specimens in the build, with the same geometry as those studied by RUS here. EBSD was provided for each raster condition in $\sim 2 \text{ mm x } 2 \text{ mm}$ total nominal areas of two different faces, with surface normals perpendicular and parallel to the BD. The EBSD measurements were performed on two orthogonal planes using a field emission scanning electron microscope operated with the following parameters: 20 kV accelerating voltage, 120 μ m aperture, 19 mm working distance, 500x magnification and dynamic focus. The multi-tile EBSD acquisition parameters were: 4x4 binning, 200 frames per second, tiles of approximately 440 μ m x 430 μ m with 5% overlap, 0.5 μ m step size and the nickel phase indexed.

2.3 Ti-6Al-4V: Electron beam powder bed fusion

Ti-6Al-4V specimens were provided by NASA Jet Propulsion Laboratory (JPL). The cylindrical specimens were printed by CalRAM⁵ on an ARCAM A2X¹ with nominal dimensions ~90 mm (height) x 16 mm (diameter) by electron beam melting (EBM). Standard EBM Ti64 powder was used for the build, as supplied by CALRAM. A standard powder bed preheat and raster strategy for Ti64 were used, with the raster strategy consisting of a hatch, outer, and inner contour regions. Three sets of AM process parameters were used to print the cylinders with identical raster strategy, denoted standard energy (SE), low energy (LE), and high energy (HE) corresponding to decreased and increased beam power. The three power settings were selected within a range of beam currents (12-18 mA) to replicate a range of common AM process parameters.

The SE printing parameters were used for both the initial ~ 15 mm and final ~ 15 mm of the build height across all the printing conditions, with the LE and HE sets of printing parameters applied for the central ~ 60 mm of the build height. Rectangular parallelepiped specimens were each extracted with EDM from each cylinder, as shown in Figure 3. The specimens selected for further study were sectioned with at least 5 mm between the specimen edge and the transition region (between processing parameters), ensuring that each

⁴Additive Manufacturing Benchmark Test Series: https://www.nist.gov/ambench

⁵California Manufacturing Technology Consulting (CMTC), a Carpenter Company



Figure 2: EBSD and sectioning strategy for the rectangular IN625 blocks printed with each raster condition. Specimens and EBSD data was provided by NIST AM Bench Test Series⁴. Inverse pole figure coloration is referenced relative to the BD. Pole figures given with scale in multiples of random distribution (MRD).

sectioned specimen contained identical processing parameters throughout. Each parallelepiped specimen was sectioned with the normal of one face parallel to the BD. The SE and HE rectangular parallelepipeds were extracted with the midpoint of their BDaligned dimension (~10.97 mm) ~50 mm from the build plate of the cylinders, while the LE specimen was extracted with the midpoint ~62 mm from the build plate. The nominal dimensions of each rectangular parallelepiped after EDM were ~7.97 mm x 10.07 mm x 10.97 mm (BD). A ±1% dimensional tolerance was considered the maximum allowable uncertainty during specimen preparation, correlating to $\leq \pm 25 \ \mu$ m following measurement with a set of vernier calipers. Specimen densities were measured as 4409 $\frac{kg}{m^3}$, 4422 $\frac{kg}{m^3}$, and 4401 $\frac{kg}{m^3}$ for the standard, low, and high energy rectangular parallelepipeds, respectively.

As shown in Figure 3, EBSD tiles were gathered to cover a nominal total area of ~ 4 mm x 7 mm of a selected specimen face of each rectangular parallelepiped, though the total area captured varied by $\pm 10\%$ between specimens. The EBSD tiles were gathered with ~ 0.5 mm spacing between the borders of each scan, to capture potential heterogeneity across the bulk of the specimen. All EBSD data was gathered using an accelerating voltage of 20 kV and current of 1.6 nA. Indexing was completed on raw pattern images



Figure 3: AM Ti64 specimens were sectioned from as-printed cylinders. Specimens were extracted 50-70 mm from the bottom of the 90 mm cylinder. EBSD scans were gathered as smaller subscans across the surface of each extracted rectangular parallelepiped specimen and aggregated to generate texture coefficients distributions. Inverse pole figure coloration is referenced relative to the BD.

with the EMSphInxEBSD package [15] prior to analysis in MTEX.

X-ray computed tomography (CT) was carried out on the as-built cylinders at NASA JPL using a voxel edge length of 17.6 μ m and geometric magnification of 7.0x. The CT data revealed a greater quantity of small-scale defects for the LE cylinder than in the SE cylinder, and the lowest quantity of small-scale defects for the HE cylinder. The defects that did exist in the HE cylinder existed at the boundary of the contour scan, and were larger than the average defects observed in the SE condition. The total calculated volume of the porosity in each cylinder was 0.008% for SE, 0.02% for LE, and 0.01% for HE.

2.4 Resonant ultrasound spectroscopy measurements

Consistent with prior studies [13, 14], RUS was performed with each AM rectangular parallelepiped specimen freely resting on piezoelectric transducers to limit external forces to those required for excitation. The setup is demonstrated in Figure 4, with two receiving transducers and one driving transducer. Increased amplitude peaks are measured across a range of frequencies to determine the first 50-75 modes. Sampling step sizes of 5 Hz were used with a dwell of 1 ms. The piezoelectric transducers, transceiver, and computer control were provided by Vibrant Corporation^{1,6}.

Broadband scans were repeated three to five times for each specimen, altering the position of the specimen/transducer between each scan. Measured frequencies were averaged across all the measured scans.

 $^{^6\}mathrm{Vibrant}$ Corporation, 8916 Adams St NE, Albuquerque, NM 87113



Figure 4: Resonant ultrasound spectroscopy testing setup with AM specimen. Each specimen freely rested under its own weight. Figure reproduced from [14].

3 Theory/Computation

3.1 Developing texture prior probability distributions with EBSD

As demonstrated in [13], variability in the input texture values directly affects the values of the single crystal elastic constants when determined from polycrystalline specimens. To increase the reliability of the determined single crystal elastic constants, texture coefficient uncertainty needs to be quantitatively incorporated into the calculation by setting the texture coefficients as random variables.



Figure 5: Distributions of each ODF coefficient (such as C_{40}^4 here) are fitted by dividing the EBSD measurement into smaller datasets and generating the ODF coefficients (C_{mn}^l) of each. This method is demonstrated for an IN625 EBSD dataset provided by the NIST AM Bench Test series⁴. The distributions of each texture parameter are used to inform the Bayesian prior of each simulation, enabling increased accuracy for the determined single crystal elastic constants.

However, the determination of arbitrary texture coefficients from the resonant frequencies results in an invariant solution (multiple numerically differentiable bulk elastic tensor representations that result in an identical set of resonant frequencies) [14, 24]. To account for the invariant representations of the texture coefficients (corresponding to the three unique sets of 180° reflections relative to each plane of symmetry in the rectangular parallelepiped) without resonant mode shape imaging, the authors previously showed that each invariant solution could be rotated to a single solution with post-processing [14]. However, concurrent solving for the texture coefficients and single crystal elastic constants results in complex parameter interdependencies and inconsistent estimates of the single crystal elastic constants, as multiple invariant solution modes are in close proximity. Therefore, the texture coefficients must be incorporated as random variables without falling victim to the multiple modes of the invariant solutions during sampling.

In order to treat the texture coefficients as random variables alongside the single crystal elastic constants, information about these texture coefficients for a given specimen is used to restrict the variables and avoid the identifiability issues when searching parameter space. This information is encoded as prior distributions during Bayesian inference. As shown in Figure 5, EBSD data was sub-divided into smaller 'tiles', with the ODF and corresponding texture coefficients generated at each tile with the MATLAB toolbox, MTEX [16, 17]. The texture coefficients across all the tiles were aggregated and used to generate distributions of each texture coefficient, which were observed to be normally distributed (as in Figure 5). The normal distribution of each coefficient from EBSD represents the possible range of each coefficient on the bulk scale, and therefore each distribution was used as the prior. Generating a distribution of each coefficient and enabling the inference to fit each value enables the use of significantly smaller EBSD datasets for the determination of the single crystal elastic constants. MATLAB scripts are included in the data supplement to generate the texture initialization conditions from EBSD data.

3.2 Calculation of resonant frequencies

The calculation of resonant frequencies is referred to as the forward model. The forward model combines the calculation of resonant frequencies from the bulk elastic constants [13, 14, 25] with a self-consistent calculation of those bulk elastic constants from the texture and single crystal elastic constants [26]. The forward model is shown in Figure 6.



Figure 6: Forward model depicting the single crystal elastic constants to be determined (left), the texture coefficients initialized from EBSD to complete the self-consistent calculation of the aggregate elastic constants (middle), and the final calculation of the resonant frequencies (right). The EBSD data overlaid on the block is not to scale.

The calculation of resonant frequencies for a rectangular parallelepiped specimen involves solving a generalized eigenvalue equation as given in Equation 1. Following [25, 27], the resonant frequencies, ω , are determined given a mass matrix, M (constructed from the specimen dimensions and density), stiffness matrix, K (constructed from the specimen self-consistent stiffness, C^{self}), and the 3-dimensional displacement vector, u. $\phi(x, y, z)$ represents the basis, with N representing the polynomial order.

$$Ku = \omega^2 M u$$

$$\phi(x, y, z) = x^n y^m z^l$$

$$n + m + l \le N$$
(1)

The computation of the stiffness matrix, K, requires the bulk elastic constants, which are calculated as the self-consistent solution, $C^{self,iso}$, given in Equation 2, as developed for tensorial texture coefficients in [26]. The self-consistent solution assumes that the polycrystalline aggregate contains a single phase of spherically shaped grains. The reference tensor, L, is defined in place of the traditional single crystal elastic constants, C^{SC} , in the orientation average, as the self-consistent solution here is defined consistent with the Hashin-Shtrikman-type bounds and assumed isotropic grain-shapes $(C^{self,iso})$ in [26]. L inherits the symmetry of C^{SC} , as it is calculated as the linear combination of the single crystal elastic constants, C^{SC} , the zeroth-order reference stiffness, $C_0^{self,iso}$, and the polarization tensor, P_0 . The polarization tensor calculation contains grain shape information, which are set as isotropic to allow the analytical determination of the calculated reference stiffness, $C_0^{self,iso}$ [13]. Without assuming isotropic grain statistics, the calculation of P_0 would require prior knowledge of the reference stiffness $(C_0^{self,iso})$, meaning an additional assumption of the stiffness of the medium would be necessary to determine the resonant frequencies during inverse solving. $C_0^{self,iso}$ is therefore calculated by solving for the con-dition that the self-consistent solution is equal to its reference stiffness, $C_0^{self,iso} = C_0$, for a given C^{SC} , with isotropic texture. f represents the ODF defined over SO(3), and $\langle \rangle$ denotes an orientation average.

$$C^{self,iso} = C_0^{self,iso} + [P_0(C_0^{self,iso})]^{-1} + [\langle f, L \rangle]^{-1}$$

$$L = [C^{SC} - C_0^{self,iso} + [P_0(C_0^{self,iso})]^{-1}]^{-1}$$

$$hd(L) \to h_{I1}, h_{I2}, H_{2,1}, H_{2,2}, H_4$$

$$f, L \rangle = h_{I1}P_1 + h_{I2}P_2 + H_{2,1} * V_{\langle 2 \rangle ij} + H_{2,2} * V_{\langle 2 \rangle ij} + H_{4,1} * V_{\langle 4 \rangle pqrs}$$
(2)

The constants h_{I1} , h_{I2} , $H_{2,1}$, $H_{2,2}$, $H_{4,1}$ are determined by the harmonic decomposition (hd) of L, as dependent on the single crystal elastic constants, C^{SC} . $V_{\langle g \rangle}$ represents the tensorial form of the texture coefficients, with g as the tensor order. The tensorial texture coefficients can be determined from the traditionally used texture coefficients, C_{mn}^{l} (where l indicates order) [28], using spherical harmonic functions [26]. The number of texture tensors that affect the specimen elasticity is dependent on the number of harmonic basis tensors for the given single crystal elastic constant symmetry, as given in [26]. The number of independent texture coefficients within each texture tensor is then dependent on the specimen symmetry, taken to be arbitrarily anisotropic (triclinic) in this work. For microscopically cubic materials, $H_{2,1} = 0$ and $H_{2,2} = 0$, meaning only the fourth order texture tensor, $V_{\langle 4 \rangle pqrs}$, with nine independent terms is needed (Equation 3) to define an arbitrary macroscopic symmetry.

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$$V_{\langle 4 \rangle pqrs} = \begin{bmatrix} V_{1111} & V_{1122} & V'_{1133} & V_{1123} & V_{1113} & V_{1112} \\ - & V_{2222} & V'_{2233} & V_{2223} & V'_{2213} & V_{2212} \\ - & - & V'_{3333} & V'_{3323} & V'_{3313} & V'_{3312} \\ - & - & - & V'_{2323} & V'_{2313} & V_{1223} \\ - & sym. & - & - & V'_{1313} & V'_{1312} \\ - & - & - & - & - & V'_{1212} \end{bmatrix}$$
(3)

Note that the parameters denoted with ' in Equation 3 are determined through linear combinations of the other parameters [14, 26]. For hexagonal materials, the second order texture tensor with five independent terms is also considered (Equation 4), given a single second order basis tensor exists.

$$V_{\langle 2\rangle ij} = \begin{bmatrix} V_{11} & V_{12} & V_{13} \\ - & V_{22} & V_{23} \\ sym. & - & V_{11} - V_{22} \end{bmatrix}$$
(4)

Again, an arbitrarily anisotropic polycrystal of hexagonal single crystalline grains is fully defined by the triclinic macrosymmetry here, with the second and fourth order texture tensors containing five and nine independent terms, respectively.

3.3 Single crystal elastic constants determined with Bayesian inference

Bayesian inference provides the capability to solve the RUS inverse problem without additional resonant mode-shape measurements [25]. Bayesian techniques provide the significant advantage of providing both parameter uncertainty and measurement uncertainty alongside the determined value of each parameter. Bayes' Theorem involves the addition of new resonant frequency observations to update prior knowledge of the independent model parameters. The posterior probability density function represents this updated knowledge as the solution to the inverse problem,

$$\pi(\Theta|\omega_n) = \frac{\pi(\omega_n|\Theta)\pi(\Theta)}{\int_{\Omega} \pi(\omega_n|\Theta)\pi(\Theta)d\Theta}$$
(5)

where Θ is the vector of the independent parameters. These independent parameters differ for each material under study here, depending on the single crystal symmetry and residual stress presence.

For SB-CoNi-10C: $\Theta^{CoNi} = [C_{11}^{SC}, C_{44}^{SC}, A, V_{\langle 4 \rangle 1111}, V_{\langle 4 \rangle 1122}, V_{\langle 4 \rangle 2222}, V_{\langle 4 \rangle 1112}, V_{\langle 4 \rangle 1113}, V_{\langle 4 \rangle 1123}, V_{\langle 4 \rangle 2212}, V_{\langle 4 \rangle 2223}, V_{\langle 4 \rangle 1223}]$: two single crystal elastic constants $(C_{11}^{SC}, C_{44}^{SC})$ and the Zener anisotropy ratio $(A = 2C_{44}^{SC}/(C_{11}^{SC} - C_{12}^{SC}))$ [29] constituting the single crystal elastic behavior, and nine 4th-order texture coefficients constituting the effect of grain orientations on elasticity for cubic materials [13, 14, 26]. Note that sampling the Zener anisotropy ratio, A, is equivalent to sampling the single crystal elastic constant, C_{12}^{SC} , such that all three independent elastic constants for cubic materials are sampled.

For IN625: $\Theta^{IN625} = [\Theta^{CoNi}, RS]$, representing the same independent parameters as SB-CoNi-10C with an additional residual stress term (RS) [14] to account for residual stress induced frequency shifts [30, 31] given the IN625 specimens were measured in the asbuilt state. The resonant frequencies of SB-CoNi-10C were measured on specimens in the stress-relieved state, and did not require the residual stress term.

For Ti64: Θ^{Ti64} is constituted by five single crystal elastic constants: $[C_{11}^{SC}, C_{33}^{SC}, C_{13}^{SC}, C_{44}^{SC}, C_{66}^{SC}]$, five 2nd order texture coefficients: $[V_{\langle 2 \rangle 11}, V_{\langle 2 \rangle 12}, V_{\langle 2 \rangle 13}, V_{\langle 2 \rangle 22}, V_{\langle 2 \rangle 23}]$, and nine 4th order texture coefficients: $[V_{\langle 4 \rangle 1111}, V_{\langle 4 \rangle 1122}, V_{\langle 4 \rangle 2222}, V_{\langle 4 \rangle 1112}, V_{\langle 4 \rangle 1113}, V_{\langle 4 \rangle 1123}, V_{\langle 4 \rangle 2212}, V_{\langle 4 \rangle 1223}]$ [26, 32]. The Ti64 powder bed preheat negated the role of residual stresses on the frequencies.

The numerator of the right hand side of Equation 5 comprises the likelihood function $\pi(\omega_n|\Theta)$ (which represents the likelihood of observing the measured resonant frequencies given Θ) and the prior $\pi(\Theta)$ (which represents prior knowledge of the independent parameters Θ). The denominator is the marginal likelihood and involves integration over

the entire parameter support, $\Omega = \{\Theta \in \mathbb{R}^3\}$. By assuming that the measurement errors are independently and identically distributed as zero-mean Gaussian distributions with variance, σ^2 , a closed form expression is obtained for the likelihood as given in [13].

An open-source, parallelized Python implementation of Sequential Monte Carlo, SMCPy⁷, was used to estimate the posterior distribution of single crystal constants. Hyperparameters were selected to ensure samples were generated from the full posterior (i.e. all modes represented) while balancing sample size with computation time. Following Section 3.1, the selection of texture coefficient priors was carried out by calculation from experimental EBSD data. For the single crystal elastic constants, improper uniform priors were chosen; i.e., $\Theta_j^{CoNi} \sim \text{Uniform}(0, 500 \text{ GPa})$ for $j = 1, \ldots, 3$. For the texture coefficients $j = 4, \ldots, 12$, normal distributions $\Theta_j^{CoNi} \sim \text{norm}(mean, std)$ were generated for each coefficient from representative EBSD data as described in Section 3.1. Though the specimen dimensions are not included as independent parameters in the inversion, the estimated single crystal elastic constants have been proven to scale in % with the geometric deviation [33]. Therefore, the maximum dimensional uncertainty (25 μ m) results in a deviation of at most 0.38% (6.5 mm x-dimension, IN625) in the single crystal elastic constants, and is neglected.

The initial particle population for all parameters was sampled from independent normal distributions, and referred to as the *proposal*. The proposal of each texture coefficient was set to the same mean value as their prior, with the standard deviation as 50% of the standard deviation of the prior. For the single crystal elastic constants, the proposal mean values were informed from the literature, \pm one standard deviation to cover the reported range of values in the literature.

Proposal normal distributions - Single crystal elastic constants (GPa)								
	C_{11}	C_{12}	C_{44}	C_{13}	C_{33}			
SB-CoNi-10C	236.4 ± 30.0	150.8 ± 20.0	134.1 ± 15.0	-	-			
IN625	243.0 ± 25.0	152.0 ± 20.0	117.8 ± 8.0	-	-			
Ti64	169.0 ± 35.0	79.0 ± 35.0	40.0 ± 10.0	62.0 ± 35.0	200.0 ± 35.0			

Table 3: Proposal distributions (normally distributed) of single crystal elastic constants for each material. \pm indicates one standard deviation on the mean. Ranges were chosen to cover the reported literature values [34, 35, 36, 37, 38, 39, 40].

The proposal normal distributions for the single crystal elastic constants of each material are given in Table 3. For SB-CoNi-10C, the means correspond to the means determined in [34] for a grown (bulk) single crystal. For IN625, the mean and standard deviation are set to cover the range of values reported in [35, 36]. For Ti64, the mean single crystal elastic constants were set as those determined in [37], with the standard deviation set to capture all the reported literature values. Note that when the Zener anisotropy ratio (for cubic materials) or C_{66} is sampled in place of another single crystal elastic constant, its proposal is calculated using the multivariate normal distibutions listed in Table 3.

In all SMC simulations, 1,800 particles were migrated through a series of target distributions that started at the prior and ended at the posterior distribution. An adaptive algorithm was used [41] that controlled the step size between target distributions using an effective sample size (ESS) threshold of 85%. Each step size was chosen such that the ESS of the updated particle population was equal to this value until the final target distribution (i.e. the posterior) was reached. To avoid particle degeneracy, a Markov Chain

⁷SMCPy Python package available open-source at https://github.com/nasa/SMCPy.

Monte Carlo (MCMC) kernel was used at each step to move particles toward the new target distribution. Each pass through the kernel involved the construction of Markov chains of length 14, retaining the 14th for the next iteration. These choices resulted in 20-35 target distributions (including prior and posterior) and corresponding computation times of 18-36 h when utilizing 10 CPU cores. Determining the single crystal elastic constants with texture uncertainty increased the computation time by \sim 30-50% compared to using fixed texture values [13], though the fixed texture calculations with inaccurate texture values often displayed excessive computation times as a result of poor convergence. All inversions used a polynomial order of 12 with 45 resonant modes.

4 Results and Discussion



4.1 SB-CoNi-10C

Figure 7: The single crystal elastic constants from the AM SB-CoNi-10C specimen are reproduced from [13] (left), where numerical differences in the fixed texture inputs generated differences in the calculated single crystal elastic constants, despite identical resonant frequencies being used for each calculation. In contrast, the single crystal elastic constants are calculated within one standard deviation of one another when the texture is freely determined with EBSD-informed priors in the calculation (right), regardless of initialization values. Literature single crystal elastic constants (black) were measured on a grown single crystal [34].

To demonstrate the advantage of allowing variability in the texture coefficients, a BDaligned SB-CoNi-10C specimen is studied. The single crystal elastic constants of this specimen were studied in [13], as determined for 'fixed' texture coefficients informed by EBSD and neutron diffraction. Note that no EBSD or neutron diffraction data was gathered for this study, rather the incorporation of freely determined texture coefficients from EBSD is studied with the EBSD and neutron diffraction data previously gathered in [13]. Here, the single crystal elastic constants are calculated from the resonant frequencies with 'freely' determined texture coefficients corresponding to calculations of the priors from EBSD in Section 3.1. Then, the single crystal elastic constants are compared to those calculated under the 'fixed' texture coefficients from [13], corresponding to tiled EBSD data, neutron diffraction data, and overfitted neutron diffraction data. Note that for the 'free' texture conditions, the mean texture coefficients are initialized from the tiled EBSD, neutron diffraction, or overfitted neutron diffraction data, while the distribution of coefficients is informed by the calculation of texture uncertainty from EBSD.

As observed in Figure 7, the final values of the single crystal elastic constants show less dependence on their initialization conditions due to the added degrees of freedom in the texture, while showing much stronger convergence. The same resonant frequencies, specimen dimensions, density, and polynomial order are used for each varied texture/ calculation. The incorporation of the texture variability from EBSD (Figures 1, 5) shifts the values of both C_{11} and A to within one standard deviation of the reference values (black), regardless of whether the mean values are initialized with EBSD or neutron diffraction. For both the neutron diffraction data and overfitted neutron diffraction data, some dependence on the initial mean is observed for C_{44} , but the solution is significantly closer to the reference values than the fixed texture condition. Therefore, this framework provides a more robust method than using fixed texture coefficients to determine the single crystal elastic constants from the resonant frequencies of AM specimens.

SB-C	SB-CoNi-10C Single Crystal Elastic Constants with Fixed Texture [13]									
	EBSD	Neutron ($R=6.8\%$)	Neutron (R= 13.2%)	Ref. Crystal [34]						
C_{11} (GPa)	238.7 ± 3.1	235.7 ± 2.4	241.0 ± 35.2	236.4 ± 1.0						
A	3.24 ± 0.07	3.76 ± 0.06	5.44 ± 0.44	3.13 ± 0.004						
C_{12}^{calc} (GPa)	154.2 ± 3.4	159.0 ± 2.6	180.7 ± 37.2	150.8 ± 0.8						
C_{44} (GPa)	137.1 ± 1.3	144.2 ± 1.0	163.3 ± 4.8	134.1 ± 0.1						
σ (kHz)	1.59 ± 0.19	1.09 ± 0.13	3.58 ± 0.41	0.08 ± 0.01						
SB-CoNi-10C Single Crystal Elastic Constants with Free Texture (Present)										
C_{11} (GPa)	239.6 ± 3.2	237.1 ± 3.5	232.9 ± 3.1	236.4 ± 1.0						
A	3.21 ± 0.25	3.45 ± 0.31	3.92 ± 0.32	3.13 ± 0.004						
C_{12}^{calc} (GPa)	154.4 ± 2.2	155.6 ± 2.2	157.8 ± 2.1	150.8 ± 0.8						
C_{44} (GPa)	136.1 ± 3.9	139.8 ± 4.6	146.4 ± 4.4	134.1 ± 0.1						
σ (kHz)	0.76 ± 0.10	0.77 ± 0.11	0.76 ± 0.10	0.08 ± 0.01						

Table 4: Single crystal elastic constants of SB-CoNi-10C specimen when initialized with different fixed-texture data (upper, as reported in [13]) or freely determined texture with priors determined by EBSD (lower). The freely determined EBSD and neutron estimates agree within one standard deviation (\pm) , while the overfitted neutron data agrees within two standard deviations. All of the free texture estimates display substantially better agreement with literature measurements on a grown single crystal (Ref. Crystal [34]), considering their uncertainties.

Comparing the calculated single crystal constants to literature reference values [34] in Table 4, the standard deviations reported in [34] are $\leq \frac{1}{3}$ of the standard deviations from the AM specimens. The lower standard deviations given in [34] are a result of the single crystal elastic constants being determined from the resonance frequencies of a grown single crystalline specimen. True single crystal specimens on the bulk scale have fewer independent parameters than the free-texture condition here, as well as significantly less noise in the actual measurement of resonant frequencies.

The simulations with texture variability were also applied to a specimen sectioned at 20°-to-BD, which was previously studied in [13]. The 20°-to-BD specimen demonstrated equally robust agreement between EBSD and neutron-diffraction informed simulations, demonstrating that the single crystal elastic constants are determinable regardless of

texture orientation. The 20°-to-BD results are available in the data supplement. 4.2 IN625



Figure 8: Single crystal elastic constants of AM IN625 comparing specimen to specimen (S1 vs S2) and raster condition (X vs XY). All the single crystal elastic constants agree within one standard deviation (error bars). The literature single crystal elastic constant values are represented by the range (black), with endpoints from [35] and [36] (no uncertainties provided). All of the specimens interrogated in this study showed agreement with the literature range within one standard deviation, except for the anisotropy ratio (A) of X_S2.

Each IN625 specimen (X_S1, X_S2, XY_S1, and XY_S2) was interrogated for their single crystal elastic constants, with texture coefficient variability informed by the EBSD scans oriented with the BD facing upward in Figure 2. These EBSD scans were each nominally 2 mm x 2 mm, demonstrating that small quantities of EBSD data are sufficient to inform the texture when texture variability is included in the calculation. Following the observed effects of residual stresses on RUS [14], a freely-determined residual stress (RS) term was included in each calculation.

As shown in Table 5, the single crystal elastic constants are within one standard deviation of one another across all parameters, with some specimen to specimen variation observed in the individual means. The specimen to specimen variability is isolated by studying the specimens S1 and S2 of each raster condition, which is observed to be less than the difference between raster conditions. The value of the RS term was zero within its uncertainty, indicating a negligible effect of residual stresses on the frequencies. While other IN625 parts were discovered to have significant residual stresses affecting RUS data [31], the builds studied here were printed with the goal of minimizing residual stresses. The parameter means \pm one standard deviation are shown in Figure 8.

Comparing the two raster conditions 'X' and 'XY', agreement is again observed within one standard deviation across all the parameters. The agreement demonstrates that the determination of single crystal elastic constants is robust to variation in the dominant

IN625 Single Crystal Elastic Constants								
	X_S1	X_S2	XY_S1	XY_S2	Ref. [35]	Ref. [36]		
C_{11} (GPa)	243.2 ± 9.0	240.0 ± 7.3	233.0 ± 9.5	231.7 ± 8.0	243.3	234.6		
A	3.13 ± 0.51	3.66 ± 0.54	3.05 ± 0.51	2.95 ± 0.36	2.72	2.83		
C_{12}^{calc} (GPa)	164.5 ± 6.7	168.7 ± 6.2	152.9 ± 7.7	150.7 ± 6.6	156.7	145.4		
C_{44} (GPa)	121.2 ± 7.8	128.6 ± 7.7	120.0 ± 7.9	118.3 ± 6.3	117.8	126.2		
RS(%)	-0.5 ± 0.9	-0.6 ± 1.0	-0.1 ± 1.1	0.1 ± 1.2	-			
σ (kHz)	1.09 ± 0.14	0.83 ± 0.10	0.98 ± 0.13	0.85 ± 0.11	-	-		

Table 5: IN625 single crystal elastic constants of AM specimens agree within one standard deviation (\pm) across raster conditions ('X', 'XY') and specimen-specimen variability (S1,S2). 'X' represents a bidirectional (180° rotation between build layers) scanning strategy while 'XY' represents a scan strategy with 90° rotations between build layers.

texture components (EBSD in Section 2.2). The convergence of the parameters validates the use of this framework for a wide variety of AM printing conditions. Relative to the range of single crystal values in the literature [35, 36], all of the specimens in this study agree within one standard deviation except for A of X_S2. Considering that the reference values in [35, 36] do not include uncertainties on the single crystal elastic constants, the agreement with literature is excellent.





Figure 9: Ti64 single crystal elastic constants calculated from specimens produced with different electron beam power settings. AM-specimen-determined single crystal elastic constants agree with range of values from literature (black) [37, 38, 39, 40] when considering two standard deviations (one standard deviation shown).

The single crystal elastic constants were determined for AM Ti64 specimens printed with high, low, and standard electron beam energies. As shown in Figure 9 and Table 6, there is agreement across all processing conditions with the range of values reported in the literature, considering two standard deviations. Note that a single standard deviation is shown in Figure 9 and Table 6 for consistency with the other single crystal estimates reported in this work.

Though all of the single crystal elastic constants fall within two standard deviations of the reported literature range, there is variability observed between the specimens with different AM processing conditions. In particular, the shear dependent single crystal elastic constants (C_{44} , C_{66}) do not agree between the different printing conditions within two standard deviations. Additionally, the range of reported values for the single crystal constants of Ti64 is broad (Figure 9), with the accurate estimates of [37] (C_{11} =169.0 GPa, C_{33} =196.0 GPa, C_{12} =62.0 GPa, C_{13} =89.0 GPa, C_{44} =43.0 GPa, C_{66}^{calc} =40.0 GPa) closest in value to the reported single crystal constants here. The values in [37] are pointwise estimates, and therefore do not have an associated standard deviation (±) or measurement error (σ) propagated through to the single crystal elastic constants.

Ti64 Single Crystal Elastic Constants									
	High Energy	Standard Energy	Low Energy	Lit. Range [37, 38, 39, 40]					
C_{11} (GPa)	166.8 ± 4.4	178.5 ± 6.8	178.2 ± 3.5	136.0 - 170.0					
C_{33} (GPa)	187.4 ± 9.9	167.7 ± 10.4	167.0 ± 6.2	163.0 - 196.0					
C_{12}^{calc} (GPa)	94.6 ± 4.8	107.8 ± 8.0	86.7 ± 3.5	62.0 - 92.0					
C_{13} (GPa)	69.0 ± 3.0	62.1 ± 3.4	73.2 ± 1.8	68.0 - 89.0					
C_{44} (GPa)	48.1 ± 1.0	48.2 ± 1.4	41.0 ± 0.5	40.0 - 52.0					
C_{66} (GPa)	36.1 ± 0.8	35.4 ± 1.3	45.7 ± 0.5	26.0 - 48.0					
σ (kHz)	0.44 ± 0.05	0.35 ± 0.04	0.30 ± 0.03	_					

Table 6: Single crystal elastic constant means and single standard deviation calculated from AM Ti64 specimens printed with different electron beam powers. Single crystal elastic constants across all AM specimens agree with range of literature values [37, 38, 39, 40] when considering two standard deviations on each value.

The difference in single crystal constants between each EBM power is likely a result of specimen to specimen variability related to porosity, phase fraction of retained β -phase, prior β -grain size, and interstitial content. The results of [10] display changes in the α phase single crystal elastic constants C_{11} and C_{12} by 41.7 GPa (31%) and 19 GPa (19%), respectively, with the inclusion of grain shape as a fitted parameter. The grain shape could not be included in the inverse calculation here, as the assumption of isotropic grain statistics is necessary to construct the inverse model of the resonant frequencies from the single crystal elastic constants (Section 3) without prior knowledge of the polycrystalline stiffness [13]. However, the substantial shifts observed in [10] support the observation of variability in the determined single crystal elastic constants of Ti64 here, as there are likely specimen to specimen microstructural differences besides the microstructural texture. Specimen to specimen variability is compounded by factors such as α -phasevariant selection during the solidification of Ti64 from its parent cubic- β phase [42]. While this phenomenon is fairly well understood relative to solidification, the effect of variant selection on texture heterogeneity and its effect on an RUS inversion through resonant mode sensitivity is completely unexplored.

The observed difference in the single crystal elastic constants of the low energy condition could stem from increased scattering with the higher volume fraction of voids as noted in Section 2.3. Despite the quantification of voids here, altering the density of the component within the resonant frequency calculation does not rigorously account for the effects of inelastic scattering on the resonant frequencies in an anisotropic medium. In fact, the effect of inelastic scattering in an anisotropic medium is not well quantified via current models and therefore could not be incorporated into the model here.

5 Conclusions

- A framework is developed to increase the accuracy of inversely determined single crystal elastic constants from the resonant frequencies of textured AM specimens. The variability of texture within the AM specimen is calculated from EBSD data and directly incorporated into the Bayesian inference of the single crystal elastic constants.
- Using texture data sourced from EBSD and neutron diffraction measurements of cobalt-nickel-base superalloy SB-CoNi-10C, the accuracy of the single crystal constants is demonstrated to significantly increase by incorporating texture coefficient uncertainty within the model (with priors determined from EBSD measurements). C_{11} and the Zener anisotropy ratio (A) of SB-CoNi-10C agree within one standard deviation of literature values, while C_{12} and C_{44} agree within two standard deviations, regardless of whether the calculation is initially given EBSD or neutron diffraction data.
- The single crystal elastic constants of Inconel 625 (IN625) are determined from the resonant frequencies of AM specimens printed under two different raster conditions, which display agreement between both raster conditions and the reported literature values within one standard deviation. $\sim 2 \text{ mm x } 2 \text{ mm}$ areas of IN625 EBSD data are shown to be sufficient to inform the texture priors of the single crystal elastic constant calculations.
- The determined single crystal elastic constants of three AM Ti64 specimens, printed with different beam powers, show agreement with the range of literature values within two standard deviations. Variability in the determined single crystal elastic constants is observed between the AM specimens with different processing parameters, indicating a susceptibility of the resonant frequencies to secondary phase and inclusion effects.

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7 Data Availability

The data used to generate the findings of this study is not provided as it is the subject of ongoing research. The SMCPy package is accessible at https://github.com/nasa/SMCPy. NIST AM Bench 2022 challenge data is accessible at https://data.nist.gov/od/id/mds2-2588. MATLAB scripts to generate the texture initialization numerics from EBSD data are provided in the data supplement.

⁸Vibrant Corporation, 8916 Adams St NE, Albuquerque, NM 87113

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