Thermo-elastic micromechanical modeling of tetragonal ZrO₂ with a herringbone microstructure inherited from the cubic phase

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Abstract

The distribution of residual stresses at the crystal scale is investigated in several random polycrystalline aggregates of zirconia. The underlying stochastic model generates tetragonal crystals forming three-dimensional herringbone microstructures, originating from cooling an initial single cubic crystal at high temperatures followed by a solid-state phase transition. The obtained microstructures are constructed following crystallographic constraints in terms of variant selection, as well as twin and band boundary orientations. This stochastic modeling approach allows generating microstructures with twin domains of various aspect ratios, embedded in several Voronoi cells as observed when the phase transition starts simultaneously from different locations in the cubic crystal. Considering the transformation strain and the anisotropic elastic and dilation properties at the crystal scale, these microstructures are solved with the spectral (FFT) full-field method for pure thermal loading (cooling). Thermal dilation has a limited effect on the residual stress field, about one order of magnitude smaller than the transformation strain, even for a cooling of 1000 °C. Normal stresses along the tetragonal crystal axes are in the order of a few GPa and proportional to the tetragonal-

Preprint submitted to Materials & Design

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ity of the zirconia crystal, except for a specific microstructure where stresses even vanish for infinite aspect ratios.

Keywords: zirconia, three-dimensional herringbone microstructure, phase transition, full-field residual stress, thermo-elasticity, stochastic geometry

1 1. Introduction

Zirconia is a well-known oxide used in numerous applications which is 2 renowned for its dual benefits: excellent thermo-mechanical properties (e.g. 3 used as a refractory material in high-temperature applications) and high ionic conductivity. Dense zirconia-based materials are usually obtained through a 5 sintering process at high temperatures or fuse cast from the liquid state. In 6 both cases, the final polycrystalline material is out-of-equilibrium, with the 7 presence of a dense network of nano-cracks together with very large residual 8 stresses (Kelly and Francis Rose, 2002; Ors et al., 2025). The coupling be-9 tween solid-state phase transitions (SPT), residual stresses and mechanical 10 response is complex. Nevertheless, for large variations of temperature, the 11 mechanical response is mainly guided by the formation of local heterogeneous 12 stress fields, due to the intrinsic highly anisotropic elastic and thermal expan-13 sion properties of the crystals constituting the material, the transformation 14 strain arising during SPT, and mechanical interactions between neighboring 15 twin domains (so-called "microstructural effects") in order to accommodate 16 the incompatible thermal and transformation deformations. 17

Due to the ability of zirconia to accommodate different atomic coordi-18 nations, pure zirconia (ZrO_2) crystallizes in different phases depending on 19 pressure and temperature. At atmospheric pressure, stress-free pure zirconia 20 solidifies into a cubic structure (denoted hereafter by 'c', space group $Fm\overline{3}m$) 21 at about 2700 °C, transforms to tetragonal one (denoted by 't', space group 22 $P4_2/nmc$) upon cooling to 2300 °C and becomes monoclinic (denoted by 23 'm', space group $P2_1/c$) at 1170 °C. In a pure zirconia single crystal, the 24 $t \to m$ SPT is of first order and it is associated with a large volume expansion 25 of about 4% (Smirnov et al., 2003). It has been described in detail in, e.g., 26 Simha (1997) and Kelly and Francis Rose (2002). In polycrystals, this $t \to m$ 27 transformation is at the origin of huge internal stresses (GPa range) promot-28 ing the development of a microcrack network into bulk specimens (Ors et al., 29 2021; Guinebretière et al., 2022; Ors et al., 2025). On the contrary, the $c \to t$ 30 SPT is a continuous second-order phase transition that can be described by 31 an alternative positive and negative shift of the oxygen atoms along the c-32 axis of the cubic cell. It means that along this axis, the oxygen coordinate is ³⁴ no longer than 0.25 but equal to $0.25 - \eta$, where η is the order parameter in ³⁵ the Landau sense (Landau and Lifshitz, 2013; Yashima et al., 1993). Because ³⁶ the $c \rightarrow t$ SPT corresponds to a decrease of symmetry, a single cubic crystal ³⁷ induces the formation of several adjacent crystals (twins) upon transition. In ³⁸ Section 2, we describe the microstructures inherited from this SPT process ³⁹ according to these crystallography rules.

The $c \to t$ SPT induces an anisotropic stress-free strain. Further cooling 40 of t crystals leads to anisotropic dilation. These two incompatible strains 41 must be accommodated by a significant elastic strain (in the order of 10^{-2}) 42 and huge stress (in the GPa range) resulting from the anisotropic elastic 43 stiffness at the crystal scale. The aim of the present paper is to make the 44 link between the stress distribution at the crystal scale and the material 45 microstructure, accounting for the crystallographic constraints of the $c \to t$ 46 SPT. For the sake of modeling the mechanical response of a polycrystalline 47 aggregate using a full-field numerical scheme, representative microstructures 48 are required. One possibility for this are phase field simulations (see, e.g., 49 Wang et al. (1995) and Mamivand et al. (2013), which stand as a powerful 50 computational tool for capturing the complex interplay of thermodynamics 51 and kinetics. However, these simulations often demand extensive compu-52 tational resources and time due to their inherent complexity and the need 53 for fine spatial-temporal resolution. In pursuit of a more expedient analy-54 sis, our research adopts a more direct modeling. Another well-established 55 approach for generating virtual, yet realistic, microstructures of polycrys-56 talline materials is given by using tessellations, i.e. a geometric partitioning 57 of a given sampling window into individual cells (i.e. twin domains) without 58 gaps. These can be obtained by employing methods from spatial stochastics 59 such as random point processes or random tessellations, see e.g. Groeber 60 et al. (2008), Redenbach and Liebscher (2015), Seitl et al. (2020) and Fu-61 rat et al. (2021). Alternatively, it is possible to start with a random, but 62 over-simplistic, microstructure, e.g., from a packing algorithm, and modify it 63 with an optimization procedure that utilizes some experimentally observed 64 characteristic, in order to acquire a more realistic structure, see Quey and 65 Renversade (2018) and Serrao et al. (2021). However, all these approaches 66 rely on three-dimensional experimental data, which is not readily available 67 for the cubic-tetragonal phase transition of zirconia due to the high tem-68 peratures involved. In the present paper, we therefore employ crystallo-69 graphic laws associated with the phase transition process to obtain realistic 70 microstructures without the need of experimental data. 71

The structure of the present paper is as follows: In Section 2 we provide a detailed description of the herringbone microstructure of $t \text{ ZrO}_2$, which

originated from a $c \operatorname{ZrO}_2$ single crystal and was subjected to the SPT. Then, 74 in Section 3, we present the microstructure model that has been developed 75 to generate 3D herringbone microstructures of the t zirconia phase. Details 76 of the numerical implementation of the spectral method used to compute 77 the thermo-mechanical response of the microstructures are presented in Sec-78 tion 4. Full-field results are shown in Section 5 and compared with the 79 analytical solution for lamella with infinite aspect ratio recalled in Appendix 80 A. The paper ends with some concluding remarks in Section 6. 81

2. Herringbone microstructure inherited from $c \to t$ phase transformation

In this section, we provide the crystallographic elements necessary for the random generation of synthetic herringbone microstructures of t zirconia (Section 3), as the 3D geometry of crystal orientations and shapes is strongly related to crystallographic relationships. This study is restricted to the case of the SPT occurring during the cooling of a c single crystal, ending with a herringbone structure made of many t crystals.

In the following, by $(hkl)_c$ and $(hkl)_t$ we denote the Miller indexes of 90 lattice planes when expressed with respect to the c and t lattices, respec-91 tively. A similar convention is used for directions, i.e. $[uvw]_c$ and $[uvw]_t$. 92 As mentioned above the tetragonal lattice is a primitive one and the \mathbf{a}_t and 93 \mathbf{b}_t lattice vectors are rotated by 45° with respect to the corresponding cubic 94 95 lattice vectors. In order to avoid additional rotations, all along the present article, the t structure will be described with respect to the multiple "tetrag-96 onal face centered" cell where the axes of the cubic and tetragonal cells are 97 in parallel of each other. The obtained tetragonal microstructure results 98 from the association of all the rotational variants allowed by the c and t99 point group relationships. It is noteworthy that the 4/mmm point group 100 is a subgroup of the $m\bar{3}m$ one (Authier, 2003). These two point groups do 101 not belong to the same crystal system, but instead are the holohedral class 102 of their crystal lattice. This transition is thus a ferroelastic one, i.e. it is 103 associated to a spontaneous change of the crystal lattice and of a variation 104 of the number of independent nonzero components of the symmetric second 105 rank tensor associated to spontaneous strain. According to Aizu (1970) it 106 can be noted by m3mF4/mmm and the number of "spontaneous nonzero 107 strain components" (called "stress-free strain components" in the following) 108 is equal to 3 in two cases, while the number of those that are independent 109 is 1 and 2 for the m3m and 4/mmm, respectively. The number of variants 110 and their relative orientations are directly induced by the loss of symmetry 111

associated with the transition from the $m\bar{3}m$ to 4/mmm point group. It is 112 obvious that this is associated with the loss of the 3-fold axis and thus it 113 generates three single crystalline states (variants). In the cubic state, the 114 3-fold axis is around the [111] direction (or any equivalent direction), that 115 is collinear to the $[111]^*$ direction (here the notation '.*' stands for the re-116 ciprocal space). This reciprocal space direction is orthogonal to any $\langle hh0 \rangle^*$ 117 directions. Thus, the 3-fold axis around the [111] direction lies in the $\{hh0\}$ 118 plane families that are oriented at 120° from each other. Considering that 119 the c_t/a_t ratio in the tetragonal state is close to 1, the twin domains ap-120 pearing through the $c \to t$ SPT are separated by twin walls belonging to a 121 $\{110\}, \{101\}, \text{ or } \{011\}$ planes. These planes are rotated by 120° with each 122 other around [111] that is the common zone axis. 123

From the experimental point of view, the formation of t microstructures 124 in doped zirconia has been described in detail by Hayakawa et al. (1986). 125 Typical examples of herringbone microstructures are shown also in Hayakawa 126 et al. (1989). There are three trivial possibilities to grow a t child phase into 127 a c parent single crystal. The two sets of lattice vectors, \mathbf{a}_t , \mathbf{b}_t , \mathbf{c}_t and \mathbf{a}_c , 128 \mathbf{b}_c , \mathbf{c}_c , stay parallel with each other, but the \mathbf{c}_t vector can align either with 129 \mathbf{a}_c or \mathbf{b}_c or \mathbf{c}_c due to the cubic and tetragonal symmetries. According to the 130 International Table For Crystallography (Authier, 2003), Hayakawa et al. 131 (1986) denotes the orientation relationship for which $\mathbf{c}_t \parallel \mathbf{a}_c$ (with $\mathbf{a}_t \parallel \mathbf{b}_c$ 132 and $\mathbf{b}_t \parallel \mathbf{c}_c$) as x variant. Similarly, a y variant has $\mathbf{c}_t \parallel \mathbf{b}_c$ (with $\mathbf{a}_t \parallel \mathbf{c}_c$ 133 and $\mathbf{b}_t \parallel \mathbf{a}_c$, and a z variant has $\mathbf{c}_t \parallel \mathbf{c}_c$ (with $\mathbf{a}_t \parallel \mathbf{a}_c$ and $\mathbf{b}_t \parallel \mathbf{b}_c$). The 134 herringbone structure consists of bands containing either x - y, x - z or y - z135 crystal sequences. 136

A schematic representation of such a microstructure is provided in Fig-137 ure 1. The x and z twins in the x - z band are separated by a $(\overline{1}01)_t$ plane, 138 the y and z twins in the y-z band by $(01\bar{1})_t$, and the two bands by the 139 $(1\overline{1}0)_t$ plane. Note the continuity of z twins across the $(1\overline{1}0)_t$ band bound-140 aries, whereas x and y twins alternate. As the three possible variants have 141 an identical probability to grow, due to the symmetries of the c structure, 142 their volume fractions in the final herringbone structure should be 1/3, as 143 also observed experimentally. Therefore, the width of z twins in the config-144 uration (called "stacking sequence" in the following) $x - z \leftrightarrow y - z$ shown in 145 Figure 1 should be half that of x and y ones as in the figure (and similarly 146 for other stacking sequences). 147

The plane at the interface between two crystals, called twin wall, can be either $(1\overline{1}0)_t$ or $(110)_t$ when there is a succession of x and y crystals. Similarly, it is either $(101)_t$ or $(\overline{1}01)_t$ for a succession of x and z orientations, and $(011)_t$ or $(0\overline{1}1)_t$ for a succession of y and z orientations. In general, a single twin wall is selected all along a band, but it can appear that the plane changes within the same band, e.g. the plane is $(101)_t$ in some part of the band but $(\bar{1}01)_t$ further away, e.g. see Figure 6 of Hayakawa et al. (1986), leading to more complex microstructures that are not considered in the present work.



Figure 1: Schematic illustration of the herringbone structure comprising many t twins denoted x, y or z according to the convention indicated in the text. The twin walls (in blue) separate x - z or y - z twin pairs that constitute the two different kinds of bands. Band boundaries (in red) separate x - y twins. The figure is a section of the microstructure normal to the [111] direction. It corresponds to the stacking sequence denoted $x-z \leftrightarrow y-z$. The loss of the 3-fold symmetry is clearly illustrated by the association of all twins.

157 3. Generation of synthetic 3D herringbone microstructures

In this section, we detail the model that has been developed for the generation of synthetic herringbone microstructures. For doing this, we have relaxed the strict crystallographic rules provided in the previous version. We still consider that only three t variants can form from the c parent crystal. Sequences of x - y, x - z and y - z twins are considered, organized in bands, but we take more degrees of freedom concerning the twin planes and band boundaries - we consider all possible planes of the {110} families.

The 3D t microstructures are generated in two steps. First some seed points are simulated in a sampling window filled with a cubic *single* crystal at high temperature. Then, the region of influence for each seed point is subdivided by inserting herringbone structures generated in accordance with the crystallographic rules described in Section 2.

More formally, consider the sampling window $\mathcal{W} = [0, 1]^3$ containing a csingle crystal with lattice parameter a_c and whose crystal axes \mathbf{a}_c , \mathbf{b}_c and \mathbf{c}_c are oriented along the axes of the used coordinate system. Based on the model parameter $n^{\text{Vo}} = 1, 2, \ldots$, which specifies the number of nucleation (i.e. seed) points for the phase transition, in total n^{Vo} seed points $\mathbf{p}_1^{\text{Vo}}, \ldots, \mathbf{p}_{n^{\text{Vo}}}^{\text{Vo}} \in \mathcal{W}$ are drawn uniformly and independently in \mathcal{W} (i.e. a realization of a binomial point process, see Chiu et al. (2013)). With these, a Voronoi tessellation (Chiu et al., 2013) with the cells $C_1^{\text{Vo}}, \ldots, C_{n^{\text{Vo}}}^{\text{Vo}} \subset \mathcal{W}$ is built. Here, the *i*-th cell C_i^{Vo} comprises all points in the sampling window \mathcal{W} that are closer to the *i*-th seed point \mathbf{p}_i^{Vo} than to any other seed point. In other words, C_i^{Vo} is given by

$$C_i^{\text{Vo}} = \{ \mathbf{x} \in \mathcal{W} : \|\mathbf{x} - \mathbf{p}_i^{\text{Vo}}\| \le \|\mathbf{x} - \mathbf{p}_j^{\text{Vo}}\| \text{ for all } j \ne i \}$$
(1)

for all $i = 1, ..., n^{Vo}$ where $\|\cdot\|$ denotes the Euclidean distance. In each 181 Voronoi cell C_i^{Vo} , a t herringbone structure is then constructed as follows: 182 As the first step, to disentangle the crystal symmetries, a coordinate system 183 is chosen at random from the 24 equivalent possibilities that are aligned 184 with the cubic crystal of the sampling window (6 possibilities to align the 185 new x-axis with the axes of the coordinate system, then 4 for the y-axis 186 and only 1 remaining for the z-axis to ensure a right-handed system). This 187 leads to (orthonormal) basis vectors $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3 \in \mathbb{R}^3$ and the lattice $L^{\text{Vo}} =$ 188 $\{(a_c i_1 \mathbf{b}_1, a_c i_2 \mathbf{b}_2, a_c i_3 \mathbf{b}_3) : i_1, i_2, i_3 \text{ integers}\}, \text{ which is used in the following.}$ 189

Next, a herringbone configuration as described in Section 2 is selected at 190 random consisting of a stacking sequence s (either $y - x \leftrightarrow z - x, x - y \leftrightarrow z - y$, 191 or $x - z \leftrightarrow y - z$), twin wall boundaries and band boundaries. Let \mathbf{n}^{bn} be the 192 unit normal vector for the band boundaries and $\mathbf{n}_{A}^{tw}, \mathbf{n}_{B}^{tw}$ be the unit normal 193 vectors of the twin walls for crystals in the two bands (denoted A and B), respectively. With this, parallel planes $P_{K_{\min}^{\mathrm{bn}}}^{\mathrm{bn}}, \ldots, P_{K_{\max}^{\mathrm{bn}}}^{\mathrm{bn}} \subset C^{\mathrm{Vo}}$ that define individual band boundaries are constructed such that they are orthogonal 194 195 196 to \mathbf{n}^{bn} and the distances to their nearest neighboring planes are equal to 197 w^{bn} for some width parameter $w^{\mathrm{bn}} > 0$ and integers $K_{\min}^{\mathrm{bn}} \leq K_{\max}^{\mathrm{bn}}$. More specifically, for the k-th band boundary plane, consider the points $\mathbf{p}_k^{\mathrm{bn}} \in P_k^{\mathrm{bn}}$ 198 199 given by 200

$$\mathbf{p}_{k}^{\mathrm{bn}} = \left\lfloor \frac{k+1}{2} \right\rfloor \mathbf{v}_{\mathrm{A}} + \left\lfloor \frac{k}{2} \right\rfloor \mathbf{v}_{\mathrm{B}} + \mathbf{p}^{\mathrm{Vo}}$$
(2)

201 with the shift vector

$$\mathbf{v}_{\mathrm{A}} = w^{\mathrm{bn}} \left(\mathbf{n}^{\mathrm{bn}} - \left\langle \mathbf{n}^{\mathrm{bn}}, \mathbf{n}_{\mathrm{A}}^{\mathrm{tw}} \right\rangle \mathbf{n}_{\mathrm{A}}^{\mathrm{tw}} \right)$$
(3)

202 for the A-bands and

$$\mathbf{v}_{\mathrm{B}} = w^{\mathrm{bn}} \left(\mathbf{n}^{\mathrm{bn}} - \left\langle \mathbf{n}^{\mathrm{bn}}, \mathbf{n}_{\mathrm{B}}^{\mathrm{tw}} \right\rangle \mathbf{n}_{\mathrm{B}}^{\mathrm{tw}} \right) \tag{4}$$

for the B-bands where $\lfloor \cdot \rfloor$ denotes the floor function, $\langle \cdot, \cdot \rangle$ denotes the scalar product and $K_{\min}^{\text{bn}} \leq k \leq K_{\max}^{\text{bn}}$. The corresponding band boundary plane P_k^{bn} is then given by

$$P_k^{\rm bn} = \left\{ \mathbf{x} \in C^{\rm Vo} : \left\langle (\mathbf{x} - \mathbf{p}_k^{\rm bn}), \mathbf{n}^{\rm bn} \right\rangle = 0 \right\}.$$
 (5)

In the following, the band $C_k^{\text{bn}} \subset C^{\text{Vo}}$ is the region enclosed by P_{k-1}^{bn} and P_k^{bn} . The values of K_{\min}^{bn} and K_{\max}^{bn} are selected such that $C_{K_{\min}^{\text{bn}}+1}^{\text{bn}}$ and $C_{K_{\max}^{\text{bn}}}^{\text{bn}}$ have a volume larger or equal to some minimum volume $v^{\min} > 0$, respectively. In the case where the Voronoi cell C^{Vo} has already a smaller volume than $2v^{\min}$, no band boundary is inserted and $C_0^{\text{bn}} = C^{\text{Vo}}$. Otherwise, P_0^{bn} is certainly present because the seed point $\mathbf{p}^{\text{Vo}} = \mathbf{p}_0^{\text{bn}}$ is always included in the Voronoi cell C^{Vo} . As the last step for constructing the bands, a type is assigned to each C_k^{bn} : if k is odd the C_k^{bn} is of type A, and of type B otherwise.

Similarly to the Voronoi cells above, every band is subsequently subdi-214 vided into individual t crystals by inserting twin walls $P_{k,L_{\min}^{tw}}^{tw}, \ldots, P_{k,L_{\max}^{tw}}^{tw} \subset$ 215 C_k^{bn} , with some integers $L_{\min}^{\text{tw}} \leq L_{\max}^{\text{tw}}$, whose normal vector is given by the considered herringbone configuration. The twin wall normal vector $\mathbf{n}^{\text{tw}} \in \mathbb{R}^3$ 216 217 is denoted \mathbf{n}_{A}^{tw} if the k-th band is of type A, and \mathbf{n}_{B}^{tw} if it is of type B. Each 218 band consists of crystals from two different crystal variants – one that is 219 unique for this type of band, and another one that is present in both types, 220 as described in the previous section. Their assignment to each band is dic-221 tated by the stacking sequence s of the herringbone configuration, e.g., for 222 $s = x - z \leftrightarrow y - z$ as in Figure 1, the z-variant is shared between all 223 bands, the y-variant belongs to the A-bands and the z-variant to the B-224 bands. The (maximum) width of a crystal is determined by whether it is 225 shared or unique. In the first case, twin walls $P_{k,\ell}^{\text{tw}}$ are separated by a distance 226 $w_{\rm s}^{\rm tw} > 0$ and by $w_{\rm u}^{\rm tw} > 0$ in the second case. For our simulations, we chose $w_{\rm u}^{\rm tw} = 2w_{\rm s}^{\rm tw}$ and $w_{\rm s}^{\rm tw} = \alpha_{\rm AR} w^{\rm bn}$ for some aspect ratio parameter $\alpha_{\rm AR} > 0$. 227 228 The ℓ -th twin plane contains the point 229

$$\mathbf{p}_{k,\ell}^{\mathrm{tw}} = \left(\left\lfloor \frac{\ell+1}{2} \right\rfloor w_{\mathrm{u}}^{\mathrm{tw}} + \left\lfloor \frac{\ell}{2} \right\rfloor w_{\mathrm{s}}^{\mathrm{tw}} \right) \mathbf{n}^{\mathrm{tw}} + \mathbf{p}_{k}^{\mathrm{bn}}$$
(6)

²³⁰ and is therefore given by

$$P_{k,\ell}^{\rm tw} = \left\{ \mathbf{x} \in C_k^{\rm bn} : \left\langle (\mathbf{x} - \mathbf{p}_{k,\ell}^{\rm tw}), \mathbf{n}^{\rm tw} \right\rangle = 0 \right\}$$
(7)

with the integer $L_{\min}^{\text{tw}} \leq \ell \leq L_{\max}^{\text{tw}}$. The crystal $G_{k,\ell}$ is given by the band boundaries P_{k-1}^{bn} and P_k^{bn} as well as the twin walls $P_{k,\ell-1}^{\text{tw}}$ and $P_{k,\ell}^{\text{tw}}$. The values of L_{\min}^{tw} and L_{\max}^{tw} are chosen such that $G_{K_{\min}^{bn}+1}$ and $G_{L_{\max}^{tw}}$ have a volume larger or equal to the minimum volume v^{\min} , respectively. For bands whose volume is lower than $2v^{\min}$, only one crystal exists, which is equal to the band. A lattice orientation is then assigned to the crystals, depending on the selected variants sequence.

Note that not all combinations of variant sequences, twin walls, and band boundaries lead to geometrically acceptable microstructures. For example, in a hypothetical $x - z \leftrightarrow y - z$ sequence with a (110) band boundaries, a ($\overline{101}$) twin wall for the x - z A band and a ($0\overline{11}$) twin wall for the y - z B band, one ends up with an unrealistic microstructure with no continuity of the z variant as it should be. Such microstructures are thus discarded in the present work.

In the following, two datasets are considered.

i) The first one, denoted by \mathcal{D}^{hs} , focuses only on the herringbone structure inside a single Voronoi tessellation cell. More precisely, it was obtained by forcing the Voronoi tessellation to have exactly one cell $C^{\text{Vo}} = \mathcal{W}$ with seed point $\mathbf{p}^{\text{Vo}} = (0, 0, 0)$. This dataset comprises 100 realization for each value of the aspect ratio $\alpha_{\text{AR}} \in \{1, 10\}$. The minimum volume parameter was set to $v^{\min} = 3 \cdot 10^{-5}$.

ii) The second dataset \mathcal{D}^{sm} consists of 400 realizations of the (unmodified) stochastic model. For this, 100 microstructures were obtained for each parameter configuration given by a value for the number of Voronoi cells $n^{\text{Vo}} \in \{4, 20\}$ and for the aspect ratio $\alpha_{\text{AR}} \in \{1, 10\}$. Again, $v^{\min} = 3 \cdot 10^{-5}$ was chosen.

In order to be able to compute the mechanical response of those microstructures with the FFT method (see next section), all realizations were discretized into $256 \times 256 \times 256$ regularly spaced voxels. Figure 2 shows three typical 3D microstructures obtained with the above model, comprising 1, 4 and 20 Voronoi cells filled with herringbone structures.

In Figure 3, some characteristics of \mathcal{D}^{sm} are presented. In Figure 3(a) the 262 mean number of twins in each realization of the stochastic microstructure 263 model is shown. As might be expected, the number of crystal variants – 264 whose type depends on the local stacking sequence – that are located in 265 both types of band are approximately twice the number of variants that are 266 only in one type of band. It is noteworthy that the aspect ratio α_{AR} has a 267 stronger influence on the number of twins than the number (and therefore the 268 size) of Voronoi cells $n^{\rm Vo}$. This fact is further illustrated when considering 269 the mean volume-equivalent diameters in Figure 3(b). 270



Figure 2: 3D visualizations of two realizations from the dataset \mathcal{D}^{hs} comprising a unique Voronoi cell $(n^{\text{Vo}} = 1)$ with (a) aspect ratio $\alpha_{AR} = 1$ and (b) $\alpha_{AR} = 10$, as well as two realizations drawn from \mathcal{D}^{sm} where (c) $n^{\text{Vo}} = 4$ with $\alpha_{AR} = 10$, and (d) $n^{\text{Vo}} = 20$ with $\alpha_{AR} = 10$.



Figure 3: (a) Plot of the mean number of twins in each realization, and (b) box plot of the volume-equivalent diameter of the twins, for each variant type and model configuration in the dataset $\mathcal{D}^{\rm sm}$.

271 4. Full-field computation

272 4.1. Computational method

Significantly high internal stress is expected in t zirconia. On the one 273 hand, this is due to the $c \to t$ phase transformation occurring at ~ 2300 °C, 274 which leads to changes in the crystal lattice parameters and resulting in 275 stress-free deformations with a marked anisotropy. The second source of 276 internal stresses is the anisotropic thermal dilation of the t phase, leading to 277 anisotropic strain during subsequent cooling. These two sources of stress-free 278 and incompatible deformation add up. In the following, the total stress-free 279 strain is denoted ε^{th} . In this work, only thermal and elastic responses are 280 considered, no plasticity nor damage is introduced. The constitutive law of 281

²⁸² the material is thus similar to a thermo-elastic one, and reads

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbf{C}(\mathbf{x}) : \boldsymbol{\varepsilon}^{e}(\mathbf{x}) = \mathbf{C}(\mathbf{x}) : \left(\boldsymbol{\varepsilon}(\mathbf{x}) - \boldsymbol{\varepsilon}^{th}(\mathbf{x})\right)$$
(8)

with \mathbf{x} denoting some position inside the herringbone microstructure and 283 $\boldsymbol{\varepsilon}^{e}, \boldsymbol{\varepsilon}^{th}$ and $\boldsymbol{\varepsilon}$ the elastic, thermal and total (i.e. thermal + elastic) strain. 284 To solve for the stress fields, we use the full-field method based on the 285 spectral method initially proposed by Moulinec and Suquet (1998) and the 286 associated open-source numerical code CRaFT (Boittin et al., 2024). In this 287 method, the computational domain \mathcal{W} is discretized into $256 \times 256 \times 256$ vox-288 els (or Fourier points). This discretization determines a regular grid in the 289 cartesian space and a corresponding grid in the Fourier space. The method 290 also requires the selection of a linear reference medium of stiffness \mathbf{C}^{0} . The 291 heterogeneous problem of a polycrystal exhibiting a different elastic stiffness 292 \mathbf{C} at each position \mathbf{x} , as in Eq. (8), is rewritten equivalently as a homoge-293 neous problem with the arbitrary homogeneous stiffness \mathbf{C}^0 and an additional 294 stress-free strain (or polarization) field $\varepsilon^{0}(\mathbf{x})$, which is unknown. The solu-295 tion is given by a convolution of the Green tensor associated to \mathbf{C}^0 with the 296 polarization field of interest. In the Fourier space, this convolution turns into 297 a direct product. The Fourier transform of the Green operator associated 298 with the reference medium can be readily calculated. Due to highly opti-299 mized numerical implementations of FFTs, the numerical efficiency of this 300 method is very high. An iterative scheme must be implemented to obtain, 301 upon convergence, the compatible strain field associate with a kinematically 302 admissible displacement field, that minimizes the average of the local strain 303 energies, under the constraint imposed by stress field balance (Suguet et al., 304 2012). 305

306 4.2. Material behavior and loading conditions

The spectral method described above is limited to computational do-307 mains submitted to periodic boundary conditions. It is only very recently 308 that a method allowing non-periodic boundary conditions has been proposed 309 (Paux et al., 2025). Therefore, periodic microstructures are often used in 310 combination with this FFT method, e.g. see Lebensohn et al. (2011). This 311 prevents from having an impact of the applied boundary conditions on the 312 mechanical fields, but at the same time this also limits the randomness of 313 the studied microstructures. Periodicity of synthetic herringbone microstruc-314 tures cannot be achieved. When computing the mechanical response of poly-315 crystalline aggregate, as a rule of thumb, specific boundary conditions are 316 often considered to have an impact on the outer shell of the computation 317

domain over a thickness of typically one twin domain. Therefore, a layer
of 20-voxels thickness at the outer surface of the computational domain has
been removed for the statistical analysis presented below. Moreover, we have
verified that the results are similar if a thicker outer shell is removed.

The results presented below are obtained for cooling. Zirconia crystal-322 lizes into a polycrystalline aggregate made of cubic crystals at about 2700 °C. 323 As cubic crystals exhibit an isotropic thermal dilation, residual stresses due 324 to cooling are not expected in the cubic domain down to 2300 °C, the tem-325 perature at which the $c \to t$ transformation is engaged. Here, we consider a 326 simple scenario in which the herringbone t microstructure is formed at once 327 at 2300 °C in a parent c stress-free single crystal. The t zirconia is then 328 further cooled down by $\Delta T = -1000$ °C, i.e. down to 1300 °C which lies still 329 higher than the $t \to m$ transformation temperature for pure zirconia. All 330 results are given at this target temperature. 331

The residual stress field at 1300 °C depends on the Bain strain during the $c \rightarrow t$ transformation, the thermal dilation of the t phase, the elastic behavior of t crystals, and of course also on the specimen microstructure.

The herringbone microstructure for t zirconia has been mostly observed for doped zirconia, as dopants such as yttrium stabilizes the t phase at lower temperatures. Lattice parameters of c and t phases depend on the dopant concentration. Here, we use the data from Mamivand et al. (2013):

$$a_c = 5.27 \text{ Å}, \quad a_t = b_t = 5.141 \text{ Å}, \quad c_t = 5.2609 \text{ Å}.$$
 (9)

339 The transformation strain for a z-variant is therefore

$$\boldsymbol{\varepsilon}^{tr} = \begin{bmatrix} -2.448 \times 10^{-2} & 0 & 0\\ 0 & -2.448 \times 10^{-2} & 0\\ 0. & 0. & -1.727 \times 10^{-3} \end{bmatrix} .$$
(10)

As for the thermal dilation of the *t* phase, several published values have been listed in Table 2 of Guinebretière et al. (2022) for bulk specimens and powders. Here, the data of zirconia powders measured by Lang (1964) between 1150 °C and 1700 °C was considered with three different compositions. It was found that the lattice parameters evolve almost linearly with temperature:

$$\frac{da_t}{dT} = 6.36 \times 10^{-5} \,\text{\AA K}^{-1} \,, \quad \frac{dc_t}{dT} = 7.57 \times 10^{-5} \,\text{\AA K}^{-1} \,. \tag{11}$$

From these values, one can already anticipate that the thermal strain, due todilation, will have a limited effect on the residual stress field. Indeed, with

³⁴⁸ $\Delta T = -1000 \,^{\circ}\text{C}$, the difference in the longitudinal thermal strain along \mathbf{a}_t ³⁴⁹ and \mathbf{c}_t directions is approximately one order of magnitude smaller than the ³⁵⁰ difference for the transformation strain.

³⁵¹ Concerning the elastic stiffness of t crystals, several values have been ³⁵² proposed in the literature, see for example Table 2 of Fadda et al. (2002). ³⁵³ The values of the components can vary significantly, for example C_{12} and C_{13} ³⁵⁴ can differ by a factor ~ 4, and the largest component C_{11} by 70%, depending ³⁵⁵ on the author. Here, we use the values measured by Kisi and Howard (1998) ³⁵⁶ and also used as reference by Zhao et al. (2011) and Mamivand et al. (2013):

$$C_{1111} = 327 \text{ GPa}, \quad C_{1122} = 100 \text{ GPa}, \quad C_{1133} = 62 \text{ GPa}, \\ C_{3333} = 264 \text{ GPa}, \quad C_{1212} = 59 \text{ GPa}, \quad C_{2323} = 64 \text{ GPa}.$$
(12)

357 5. Results

358 5.1. Results for a single Voronoi cell

In this section, we start with the microstructures from the simpler dataset 359 \mathcal{D}^{hs} , i.e. those for which only a single Voronoi cell was used (i.e. $n^{Vo} = 1$) 360 as in Figures 2a and 2b. Each cell is defined by a number of geometri-361 cal/crystallographical features, namely a stacking sequence, the twin planes 362 inside the bands and the band boundary plane. Three different stacking 363 sequences are possible, named as $y - x \leftrightarrow x - z, x - y \leftrightarrow y - z$ and 364 $x - z \longleftrightarrow z - y$ where the repeated variant name corresponds to the variant 365 shared by the two bands. To indicate the twin planes and the band bound-366 ary orientation, we use a notation such as $y \xrightarrow{(011)} x \xleftarrow{(110)} x \xrightarrow{(101)} z$ indicating a 367 (011) twin planes between y and x variants in the first band, a (101) twin 368 plane between variants x and z in the second band, and a plane (110) as 369 band boundary. In total, 18 different combinations are possible, 3 possible 370 stacking sequences and for each stacking sequence 6 possible permutations 371 of plane indices, all listed in Table 1. Evidently, as the initial c crystal ex-372 hibit cubic symmetries, and since we are considering only isotropic loadings 373 (thermal loading) of the herringbone t microstructures, some of these 18 mi-374 crostructures generate similar stress and strain fields that are only rotated 375 by 90° with respect to one of the cubic axes. This is for example the case for 376 $y \stackrel{(110)}{-} x \stackrel{(011)}{\longleftrightarrow} x \stackrel{(101)}{-} z$ and $x \stackrel{(110)}{-} y \stackrel{(101)}{\longleftrightarrow} y \stackrel{(011)}{-} z$. Accounting for these symme-377 tries, we end up with 6 different microstructures and 6 different mechanical 378 responses. Symmetrically equivalent microstructures are grouped by a color 379 code in Table 1. 380

Table 1: Mean value of the normal stress σ_c , expressed in MPa, for various microstructures. Full-field results for the aspect ratios $\alpha_{AR} = 10$ and $\alpha_{AR} = 1$ and a single Voronoi cell. Exact results for rank-2 laminates, corresponding to infinite aspect ratio ($\alpha_{AR} = \infty$) are also provided. The color code indicates the microstructures with similar thermomechanical response.

	0	-200	-540		1883.4	.1850	-881		1939.1	-1992	-2625		2129.9	-2156	-2630		2137.4	-2047	-1083		410.5	-529	-749
$x\stackrel{(101)}{-}z\stackrel{(110)}{\longleftrightarrow}z\stackrel{(011)}{-}y$	0	-32	-700	$\stackrel{(0)}{ ightarrow} \stackrel{(101)}{z} \stackrel{(101)}{-} y$	-402.8 -3	-376 -	-735	$\stackrel{1}{\rightarrow} z \stackrel{(011)}{-} y$	130.1 -:	-130	-1372	$x \stackrel{(011)}{-} z \stackrel{(101)}{\longleftrightarrow} z \stackrel{(110)}{-} y$	-3415.4 -5	-3166	-1656 -	$x \stackrel{(110)}{-} z \stackrel{(011)}{\longleftrightarrow} z \stackrel{(101)}{-} y$	-618.0 -5	-755 -	-1560	$\stackrel{(1)}{\rightarrow} z \stackrel{(110)}{-} y$	-3841.7 -	-3514	-1798
	0	-32	-700	$x \stackrel{(011)}{-} z \stackrel{(11)}{\leftarrow}$	-402.8	-376	-735	$\begin{pmatrix} (110) \\ - z \end{pmatrix} \xrightarrow{(10)}$	-3841.7	-3514	-1798		-618.0	-755	-1560		-3415.4	-3166	-1656	$\begin{pmatrix} 101 \\ - z \end{pmatrix} \stackrel{(01)}{\leftarrow}$	130.1	-130	-1372
	0	-200	-540		-1883.4	-1850	-881	r	-410.5	-529	-749		-2137.4	-2047	-1083		-2129.9	-2156	-2630	G	-1939.1	-1992	-2625
$x \stackrel{(110)}{-} y \stackrel{(101)}{\longleftrightarrow} y \stackrel{(011)}{-} z$	0	-200	-540		-410.5	-529	-749	$x \stackrel{(101)}{-} y \stackrel{(110)}{\longleftrightarrow} y \stackrel{(011)}{-} z$	-1939.1	-1992	-2625	$x \stackrel{(101)}{-} y \stackrel{(011)}{\longleftrightarrow} y \stackrel{(110)}{\longrightarrow} z$	-2137.4	-2047	-1083	$x \stackrel{(011)}{-} y \stackrel{(110)}{\longleftrightarrow} y \stackrel{(101)}{-} z$	-2129.9	-2156	-2630	$\stackrel{(11)}{ ightarrow} \stackrel{(110)}{-z}$	-1883.4	-1850	-881
	0	-32	-700	$\stackrel{(1)}{\rightarrow} y \stackrel{(101)}{-} z$	-3841.7	-3514	-1798		130.1	-130	-1372		-618.0	-755	-1560		-3415.4	-3166	-1656		-402.8	-376	-735
	0	-32	-700	$x \stackrel{(110)}{-} y \stackrel{(01)}{\leftarrow}$	130.1	-130	-1372		-3841.7	-3514	-1798		-3415.4	-3166	-1656		-618.0	-755	-1560	$x \stackrel{(011)}{-} y \stackrel{(10)}{\leftarrow}$	-402.8	-376	-735
	0	-200	-540		-1939.1	-1992	-2625		-410.5	-529	-749		-2129.9	-2156	-2630		-2137.4	-2047	-1083		-1883.4	-1850	-881
$y \stackrel{(110)}{-x} \stackrel{(011)}{\longleftrightarrow} x \stackrel{(101)}{-z}$	0	-200	-540	$\stackrel{(01)}{\rightarrow} x \stackrel{(011)}{-z}$	-410.5	-529	-749	$y \stackrel{(101)}{-} x \stackrel{(011)}{\longleftrightarrow} x \stackrel{(110)}{-} z$	-1883.4	-1850	-881	$y \stackrel{(101)}{-} x \stackrel{(110)}{\longleftrightarrow} x \stackrel{(011)}{-} z$	-2129.9	-2156	-2630	$y \stackrel{(011)}{-} x \stackrel{(101)}{\longleftrightarrow} x \stackrel{(110)}{-} z$	-2137.4	-2047	-1083		-1939.1	-1992	-2625
	0	-32	-700		-3841.7	-3514	-1798		-402.8	-376	-735		-3415.4	-3166	-1656		-618.0	-755	-1560	$y \stackrel{(011)}{-x} \stackrel{(110)}{\longleftrightarrow} x \stackrel{(101)}{\longrightarrow} z \stackrel{(101)}{-z}$	130.1	-130	-1372
	0	-32	-700	$y \stackrel{(110)}{-} x \stackrel{(110)}{\leftarrow}$	130.1	-130	-1372		-402.8	-376	-735		-618.0	-755	-1560		-3415.4	-3166	-1656		-3841.7	-3514	-1798
	0	-200	-540		-1939.1	-1992	-2625		-1883.4	-1850	-881		-2137.4	-2047	-1083		-2129.9	-2156	-2630		-410.5	-529	-749
	$\alpha_{AR}=\infty$	$\alpha_{AR} = 10$	$\alpha_{AR} = 1$		$\alpha_{AR}=\infty$	$\alpha_{AR} = 10$	$\alpha_{AR} = 1$		$\alpha_{AR} = \infty$	$\alpha_{AR} = 10$	$\alpha_{AB} = 1$	4	$\alpha_{AR} = \infty$	$\alpha_{AR} = 10$	$\alpha_{AR} = 1$		$\alpha_{AR} = \infty$	$\alpha_{AR} = 10$	$\alpha_{AR} = 1$		$\alpha_{AR} = \infty$	$\alpha_{AR} = 10$	$\alpha_{AR} = 1$

In the following, we discuss the results from the full-field computations, 381 performed for two aspect ratios, $\alpha_{AR} = 10$ and $\alpha_{AR} = 1$. We expressed all 382 stress tensors in a reference frame attached to the t crystal lattice. Here, 383 we will mostly concentrate on the normal stress components denoted σ_a, σ_b , 384 σ_c . For example, σ_c is the normal stress along the *c*-axis of a *t*-crystal, i.e. 385 acting on a $(001)_t$ lattice plane along the direction $[001]_t$. For each generated 386 microstructure, we have computed the stress distributions in twin domains 387 with a given lattice orientation (i.e. same variant) and a given band, and 388 estimated the mean and dispersion values of these distributions. The results 389 for the mean normal stress σ_c within each variant are reported in Table 1. 390 Exact results for rank-2 laminates, corresponding to infinite aspect ratio 391 $(\alpha_{AB} = \infty)$ are also provided, see Appendix A. 392

(i) It can be remarked that the obtained mean stress values for σ_c are huge. In all microstructures except for the ones indicated in the first line of the table (yellow cells), there is at least one variant for which σ_c lies in the GPa range, and up to -3.8 GPa. In general, only non-positive values (compressive stress) are obtained.

(ii) All mean normal stress components are reported in Table 2 for the case $\alpha_{AR} = 10$ and for 6 representative microstructures (the 12 remaining ones can be obtained by symmetry operations as discussed above). Similar to σ_c , the values for σ_a and σ_b also lie in the GPa range, except for the yellow cells. This time, however, positive (tensile) stress values, up to +3.2 GPa, are also obtained.

(iii) For the sake of conciseness, shear stress values are not given explicitly here. They have been found to be significantly smaller (in absolute value) than normal stresses, generally in the range of tens of MPa. The largest obtained value for $\alpha_{AR} = 10$ is 450 MPa.

(iv) According to Table 1, the aspect ratio of the t lamellae plays an important role in the stress distribution. Results for $\alpha_{AR} = 1$ and $\alpha_{AR} = 10$ show some similarities but the obtained values for σ_c can be quite different.

(v) Note that in Table 1 some microstructures exhibit similar distribution 412 of σ_c beyond the basic symmetry operations discussed above. This is, 413 for example, the case for the gray and green cells, as well as for the 414 orange and blue ones. For these microstructures, however, σ_a and σ_b 415 do not match together (see Table 2) for a given variant, but we find the 416 same stress values in other variants. The values are simply permuted. 417 For the yellow and red cells, we find the same values for σ_a and σ_b 418 belonging to the variant not shared by both bands. These values are 419

Table 2: Mean value of the normal stresses components σ_a , σ_b and σ_c , expressed in MPa, for each set of equivalent microstructures. Full-field results for an aspect ratio $\alpha_{AR} = 10$ and a single Voronoi cell. The color code is similar than for Table 1.



simply swapped. We also find the same swapped sets of values for grayand green cells.

When looking into the details of the stress distributions within the various microstructures, it is apparent that there are basically three different cases:

1. For some microstructures, a bimodal stress distribution is obtained within the whole microstructure. This is the case for the yellow and red cells in Table 1, where the twin domains belonging to the variant shared by the two bands on one side, and belonging to the two other variants on the other side, exhibit the same mean stress value σ_c .

429 2. For other microstructures (blue and orange cells in Table 1), the mean 430 stress in twin domains belonging to the variant shared by both bands 431 are significantly different, whereas in the other two variants, values of 432 σ_c are almost identical.

⁴³³ 3. For the remaining configurations (gray and green), four significantly ⁴³⁴ different mean values of σ_c are obtained for each variant in each band. In the case of $\alpha_{AR} = 10$, for example in $y \stackrel{(110)}{-} x \stackrel{(101)}{\longleftrightarrow} x \stackrel{(011)}{-} z$, the mean stress in twin domains belonging to variant x can be relatively small inside the band containing also the variant y (namely -0.13 GPa), but huge (in absolute value) inside the other band containing also the variant z (namely -3.5 GPa).

Note that the classification above depends on the stress component considered (Table 2). For example in $y \stackrel{(101)}{-} x \stackrel{(011)}{\longleftrightarrow} x \stackrel{(110)}{-} z$, the same value for σ_c is found within the variant x for both bands, but significantly different values for σ_a and σ_b in the same variant between both bands.



Figure 4: Distribution of σ_c in microstructures $y \stackrel{(101)}{-} x \stackrel{(011)}{\longleftrightarrow} x \stackrel{(110)}{-} z$ (left) and $y \stackrel{(011)}{-} x \stackrel{(110)}{\longleftrightarrow} x \stackrel{(110)}{\longrightarrow} x \stackrel{(101)}{\longrightarrow} x \stackrel{$

Figure 4 illustrates the observations above. It shows the 3D field of σ_c for a microstructure $y \xrightarrow{(101)} x \xleftarrow{(110)} x \xrightarrow{(110)} z$ corresponding to case 1 (bimodal distribution of σ_c), and a microstructure $y \xrightarrow{(011)} x \xleftarrow{(110)} x \xrightarrow{(101)} z$ for which 4 different stress values arise (case 3), both with $\alpha_{AR} = 10$. The probability

densities of the residual stress are also provided. Here, the stress hetero-448 geneity inside each twin domain is small, leading to well distinct and narrow 449 peaks in the stress distribution. In $y \xrightarrow{(101)} x \xleftarrow{(011)} x \xrightarrow{(110)} z$, the x variants of 450 both bands show the same stress level. This is also the case for variants y451 and z. Contrarily, for $y \xrightarrow{(011)} x \xleftarrow{(110)} x \xrightarrow{(101)} z$, the 4 variants exhibit different 452 stress states, and in particular the stress in the x variant in both bands is 453 significantly different $(-3.5 \,\text{GPa} \text{ and } -0.13 \,\text{GPa})$. These results show that 454 in such herringbone microstructures, the mean stress in twin domains with 455 similar crystallographic orientation is not guided essentially by their lattice 456 orientation as often encountered in polycrystalline aggregates e.g. see Gu 457 et al. (2017) and Purushottam Raj Purohit et al. (2021), but crystal stresses 458 are highly dependent on the local crystal arrangement. 459



Figure 5: Probability density functions averaged over the 18 possible microstructures with $\alpha_{AR} = 10$ and $n^{\text{Vo}} = 1$ for (a) σ_a , (b) σ_b , and (c) σ_c .

To go one step further in the analysis of the statistical distribution inside the constituting crystals, in Figure 5 the probability density of σ_a , σ_b and σ_c is shown for an aspect ratio $\alpha_{AR} = 10$ when considering all possible microstructures indicated in Table 1. The main findings are:

- (i) The distributions of σ_a and σ_b turn out to be similar, due to the tetragonal symmetry of the crystal lattice.
- (ii) The distributions of σ_a and σ_b show 4 peaks, whereas that of σ_c has only 3.

(iii) These three distributions are extremely broad with widths between $-4 \,\mathrm{GPa}$ and $4 \,\mathrm{GPa}$.

These results highlight again the huge impact of the local crystallographic and morphologic environment on the stress state of a given crystal in the whole microstructure.

473 5.2. Influence of the aspect ratio of twin domains

We have also investigated the impact of the twin domain aspect ratio on the resulting distribution of residual stress in the various microstructures. Examples of microstructures with aspect ratios $\alpha_{AR} = 1$ and $\alpha_{AR} = 10$ are shown in Figure 2a and 2b, respectively.



Figure 6: Probability density functions of σ_c for the microstructure $y \stackrel{(011)}{-} x \stackrel{(110)}{\longleftrightarrow} x \stackrel{(110)}{-} z$ with $n^{\text{Vo}} = 1$ for the aspect ratios (a) $\alpha_{AR} = 1$ and (b) $\alpha_{AR} = 10$. The arrows indicate which variant the distribution corresponds to.

The probability density of σ_c for the sequence $y \xrightarrow{(011)} x \xleftarrow{(101)} x \xrightarrow{(110)} z$ is shown in Figure 6, for both aspect ratio. Increasing the aspect ratio from 1 to 10 very clearly leads to a narrowing of the stress distribution in all variants. Apparently, for $\alpha_{AR} = 1$, the distribution of σ_c in the y and z variants are well separated (by ~ 2 GPa), but for $\alpha_{AR} = 10$ they are almost overlapping. Conversely, the x variants in both bands behave very similarly for $\alpha_{AR} = 1$, but are clearly distinct for $\alpha_{AR} = 10$.

The case $\alpha_{AR} = 1$ was investigated mostly to track the effects of drastic 485 changes in microstructures. It probably departs from real microstructures 486 due to exhibiting a very extreme morphology. For example, the experimental 487 observations (electron micrograph) of Hayakawa et al. (1986) show aspect 488 ratio more in the range $\alpha_{AR} \sim 10 - 20$, i.e. similar to microstructures 489 investigated in Section 5.1. On the other hand, this shows that the procedure 490 for microstructure generation, described in Section 3, is robust and capable 491 of constructing highly different microstructure types. 492

Herringbone microstructures with very large aspect ratio can hardly be studied numerically, as this would require a much larger computational domain for the FFT solver. However, microstructures with infinite aspect



Figure 7: (a) Schematic representation of a rank-1 laminate with normal \mathbf{n} , made of two materials with elastic stiffness and stress-free strain \mathbf{C} and ε^0 , respectively. (b) In the rank-2 laminate with normal \mathbf{n} , each layer is itself a rank-1 laminate with effective stiffness and effective stress-free strain $\tilde{\mathbf{C}}$ and $\tilde{\varepsilon}^0$.

ratio $(\alpha_{AR} \to \infty)$ are easy to handle through the analytical solution for 496 thermo-elastic laminates. The microstructure of such a periodic composite 497 is illustrated in Figure 7. A rank-1 laminate is composed of a succession 498 of planar, parallel, infinite and perfectly bonded layers. Each layer has a 499 different elastic stiffness and stress-free strain. The *exact* effective stiffness 500 and effective stress-free strain of such a composite can be easily calculated. 501 A rank-2 laminate can be constructed similarly by piling-up layers made of 502 rank-1 laminates. Continuing the same process, it is possible to construct 503 rank-n laminates, up to infinite order as in Francfort and Murat (1986) and 504 Idiart (2007). The elastic response of rank-1 laminates has been investigated 505 first by Backus (1962). The thermo-elastic response has received much less 506 attention. In Appendix A, we extend the analytical solution given in Milton 507 (2002) by providing a compact expression of the residual stress field. A well-508 known exact result concerning the thermo-elastic response of laminates is 509 that the stress and strain fields inside each layer are uniform, and therefore 510 the stress distributions shown above for finite α_{AR} values (Figures 4, 5 and 511 6) become Dirac shaped for $\alpha_{AR} \to \infty$. 512

The interest for such a rank-2 laminate structure within the present study 513 is twofold. First, it resembles the herringbone structure described in Sec-514 tion 2, with the finest lamellas representing the twinning process, and the 515 largest (rank-2) lamination the large bands observed in herringbone struc-516 tures. And second, if at each stacking step, one piles up a very large number 517 of thin layers so that the physical scale of the whole laminate is much larger 518 than the one of each layer, then the analytical solution provided in Appendix 519 A is *exact*. This condition implies that the aspect ratio of the layers, at each 520 stacking step, is infinite. 521

We have thus constructed rank-2 laminates for herringbone microstructures following the same crystallographic rules as described in Section 3. The



Figure 8: Effect of the tetragonality c_t/a_t on the stress component σ_c in one of the x twin domains for the microstructure $y \xrightarrow{(110)} x \xleftarrow{(101)} x \xrightarrow{(011)} z$ (gray curves), accounting for SPT only (continuous line) and for SPT plus cooling (dashed line). For $y \xrightarrow{(110)} x \xleftarrow{(011)} z$ (yellow curve), the value of σ_c in all twin domains remains zero regardless of tetragonality, dilation coefficients of the t phase and cooling range. Results from the rank-2 analytical solution corresponding to $\alpha_{AR} \to \infty$ and $n^{Vo} = 1$.

values obtained for σ_c are indicated in Table 1.

(i) One can observe that the difference in σ_c between the cases $\alpha_{AR} = 10$ (mean values of σ_c) and $\alpha_{AR} \to \infty$ (exact values of σ_c) are rather small, generally of the order of a few tens of MPa, the largest difference being 0.33 GPa.

(ii) The 3 microstructures highlighted in yellow in Table 1 turn out to be 529 very specific. Already in the cases $\alpha_{AR} = 1$ and $\alpha_{AR} = 10$, much lower 530 σ_c values were found compared to other microstructures. In the case 531 $\alpha_{AR} \to \infty$, one obtains that σ_c is strictly zero, and we have checked that 532 all other stress components also vanish. These specific microstructures 533 thus correspond to a case for which both SPT and anisotropic ther-534 mal dilation of the t phase do not lead to any residual stress, thus no 535 stored elastic energy, and also no reason for the appearance of cracks. 536 It can be checked that this corresponds to configuration for which both 537 transformation strain and thermal strain are compatible, and therefore 538 there is no need for additional elastic accommodation during the cool-539 ing process. Also, interestingly, these 3 microstructures correspond to 540 the experimental ones described in Section 2, based on the possible 541 twinning planes associated with the crystal structures. 542

(iii) We have verified with the analytical solution for the laminate that
 the sign of the Miller indices used to describe the twin planes and

band boundaries has no effect on the stress field, i.e. calculating the response of a microstructure comprising e.g. a (110) plane or a ($\overline{1}10$) plane gives exactly the same results. The same behavior has also been found with the full-field numerical approach, even if the microstructures are geometrically different. This is why we have removed the sign of all Miller indices in Tables 1 and 2.

(iv) Using the analytical solution for laminates, one can also easily estimate 551 the relative importance of the transformation strain associated with the 552 SPT and thermal dilation in the build-up of the residual stress field. 553 Performing calculations accounting for the SPT either with cooling 554 $(\Delta T = -1000 \,^{\circ} \,\mathrm{K})$ or without cooling $(\Delta T = 0 \,^{\circ} \,\mathrm{K})$, both resulting 555 residual stress fields are very close. All stress components in the case 556 that included cooling are slightly smaller by about 5% (in absolute 557 value) than without cooling. The residual stress field is thus essentially 558 governed by the transformation strain. 559

(v) Among all material parameters listed in Section 4.2, all results pre-560 sented above do not depend directly on the lattice parameters, nor on 561 the dilation coefficients. Only the tetragonality c_t/a_t and the ratio of 562 the dilation coefficients along \mathbf{c}_t and \mathbf{a}_t of the t phase come in play. 563 The lattice parameter of the c phase does not have any influence on 564 the stress field for the calculation conditions adopted here. The tetrag-565 onality is a particularly important parameter as it is routinely adjusted 566 by adding dopants such as yttria in order to stabilize the t phase down 567 to room temperature, see e.g. Krogstad et al. (2011). Figure 8 shows 568 the effect of the tetragonality on the value of σ_c in one illustrative 569 microstructure $y \stackrel{(110)}{-} x \stackrel{(101)}{\longleftrightarrow} x \stackrel{(011)}{-} z$, when the zirconia has been sub-570 mitted to SPT only (thus forming the herringbone structure) or when 571 it has been submitted to SPT and cooling ($\Delta T = -1000$ °C) as above. 572 This figure illustrates the small effect of thermal cooling compared to 573 the SPT, i.e. a constant difference of 216 MPa being found between 574 both curves. For both cases, the residual stress field evolves linearly 575 with c_t/a_t , and a similar linear response (not shown) is obtained when 576 modifying the ratio of the dilation coefficients of the t phase. Again, 577 the specific $y \xrightarrow{(110)} x \xleftarrow{(011)} x \xrightarrow{(101)} z$ microstructure (yellow in Tables 1 578 and 2) shows a very specific behavior with vanishing residual stress (all 579 components in all twin domains), regardless of tetragonality, cooling 580 range, and ratio of dilation coefficients for the t phase. 581

582 5.3. Microstructure comprising several Voronoi cells

Finally, we have investigated the effect of having several Voronoi cells in 583 the computational domain, each of which contains a herringbone structure of 584 a random configuration. These generated microstructures match the experi-585 mental ones more closely. The different Voronoi cells may reflect a process in 586 which the phase transition starts simultaneously at different positions within 587 a large parent c crystal at high temperature. Several herringbone microstruc-588 tures thus grow concurrently and meet at some point where a new boundary 589 is formed between the individual herringbone structures. These boundaries 590 are modeled by the facets of the Voronoi cells described in Section 3. 591



Figure 9: Box plots describing the distributions of σ_c in the Voronoi cells comprising the sequence $y \stackrel{(101)}{-} x \stackrel{(011)}{\longleftrightarrow} x \stackrel{(110)}{-} z$ for nine generated microstructures with $\alpha_{AR} = 10$ and $n^{\text{Vo}} = 20$ Voronoi cells. The colors correspond to the variants (i.e. x, y and z) as indicated by the arrows.

We focus in the following on the stacking sequence $y \stackrel{(101)}{-} x \stackrel{(011)}{\longleftrightarrow} x \stackrel{(110)}{-} z$ 592 with an aspect ratio $\alpha_{AR} = 10$. In Figure 9, nine generated microstructures 593 are considered each comprising $n^{\text{Vo}} = 20$ Voronoi cells. For these, box plots 594 of the distribution of σ_c within the Voronoi cells containing the sequence 595 $x \stackrel{(011)}{\longleftrightarrow} x \stackrel{(110)}{-} z$ are shown . It is apparent that quite strong fluctuations y -596 occur in all the 3 variants from one microstrostructure to another, not only 597 for the mean values of σ_c , but also for the dispersion of the distributions. For 598 example, the standard deviation of σ_c can vary from 100 MPa to 600 MPa in 599 variant y, depending on the microstructure. 600

Figure 10 shows the distributions of σ_c , for the same sequence, still in microstructures comprising 20 Voronoi cells, but now as a statistical average over many replications from the stochastic microstructure model. These



Figure 10: Probability density functions of σ_c in one Voronoi cell comprising the sequence $y \stackrel{(101)}{-} x \stackrel{(011)}{\longleftrightarrow} x \stackrel{(110)}{\longrightarrow} z$ averaged over many generated microstructures with $\alpha_{AR} = 10$ and $n^{\text{Vo}} = 20$ Voronoi cells.

distributions can be compared to that given in Figure 4a which was calculated for a microstructure comprising a single Voronoi cell for the same sequence. Clearly, the presence of boundaries randomly delimiting two specific sequences of variants significantly increases the spread of the distributions of residual stress.

A general conclusion of this section is that when different herringbone structures grow simultaneously in the same initial *c* crystal, the residual stress field is globally of higher intensity, and stress distributions are broader compared to the case with a single Voronoi cell (i.e. a single nucleation point of the SPT). This is due to the additional strain incompatibilities between all herringbone structure, compared to the case where only one Voronoi cell is present.

(110)However, there is still a very specific case with the microstructures y' – 616 $x \stackrel{(011)}{\longleftrightarrow} x \stackrel{(101)}{-} z$ highlighted in yellow in Table 1. For $\alpha_{AR} \to \infty$, besides 617 vanishing residual stresses for the case of a single herringbone structure as 618 found in Section 5.2, the effective stress-free strain $\tilde{\varepsilon}^0$ of such microstructures 619 turns out to be isotropic (strain value is found to be -2.36×10^{-2} i, with i 620 the second rank isotropic tensor). Therefore, when all Voronoi cells of the 621 microstructure contain such a sequence, even oriented differently, the final 622 residual stress field still vanishes, with no elastic energy stored, regardless of 623 the position and orientation of the boundary between the different herring-624 bone structures (i.e. facets of the Voronoi tessellation) because the effective 625 stress-free strain inside each Voronoi cell is equal and isotropic, thus com-626

patible. This might be the reason why the Laue microdiffraction patterns
measured at high temperature in pure tetragonal zirconia in Purushottam
Raj Purohit et al. (2024) seem to indicate very little lattice distortion.

630 6. Concluding remarks

In this work, we have investigated the residual stress field that may arise 631 during the $c \to t$ phase transition and thermal cooling in zirconia. For doing 632 this, we have proposed a new scheme for the generation of three-dimensional 633 herringbone microstructures that are representative of the tetragonal phase. 634 These synthetic microstructures can contain one or more herringbone struc-635 tures, each in a separate Voronoi cells, and the individual twin domains 636 inside these structures can exhibit various aspect ratios. Such microstruc-637 tures have been investigated numerically by a spectral method for two twin 638 domain aspect ratios, $\alpha_{AR} = 1$ and $\alpha_{AR} = 10$. The exact behavior in the 639 case of infinite twin domain aspect ratio has also been provided based on the 640 analytical solution for rank-2 thermo-elastic laminates. The main results can 641 be summarized as follows: 642

(i) 18 individual herringbone microstructures have been generated and in vestigated. They can be grouped into 6 different sets each containing
 3 similar microstuctures, which, due to the isotropic thermal loading,
 differ only by symmetry operations of the initial c crystal.

(ii) In all investigated cases – except the specific ones described below – normal residual stresses in each type of twin domain reach huge values, with mean values lying in the range [-3.8 GPa : +3.8 GPa]. Shear stresses are found to be much smaller by one order or magnitude. The mean residual stress along the c axis, σ_c , is always negative, while the mean values of σ_a and σ_b are mostly positive, although some negative values are also found for some specific microstructures.

(iii) The stress distribution over the whole microstructure can have 2, 3 654 or 4 well-defined maxima, depending on the microstructure type. In 655 particular, twin domains of the same variant can exhibit significantly 656 different residual stress levels depending on their local environment, i.e. 657 to which band they belong. A consequence of this result is that, if local 658 stress measurements are performed once, e.g., using high resolution 659 EBSD (Plancher et al., 2017) or Laue microdiffraction (Purushottam 660 Raj Purohit et al., 2024), the interpretation of the results will require 661 thorough knowledge of the local specimen microstructure. 662

(iv) The effect of thermal expansion is negligeable compared to the one of the transformation strain (~ 5%) even for a significant cooling of $\Delta T = -1000$ ° K.

(v) Microstructures with twin domains having a small aspect ratio ($\alpha_{AB} =$ 666 1) globally exhibit similar features than the ones with higher aspect 667 ratio ($\alpha_{AR} = 10$), but show a larger spread of the stress distributions. 668 (vi) When several herringbone structures live together in a single microstruc-669 ture, represented in this work by several Voronoi cells, the distributions 670 of the residual stress field remains globally similar to those for a sin-671 gle herringbone structure, but with broader stress distributions. We 672 expect that the stress distributions in a specimen of t zirconia arising 673 from a polycrystal of c zirconia (at high temperature), will be similar 674 to those investigated here and comprising many Voronoi cells. 675

(vii) Finally, three very specific microstructures have been identified, namely 676 $y \xrightarrow{(110)} x \xleftarrow{(011)} x \xrightarrow{(101)} z, \ x \xrightarrow{(110)} y \xleftarrow{(101)} y \xrightarrow{(011)} z \text{ and } x \xrightarrow{(101)} z \xleftarrow{(110)} z \xrightarrow{(011)} y.$ 677 In the case of infinite aspect ratio, they all lead to isotropic effective 678 stress-free strain and no residual stress at the twin domain level, re-679 gardless of the number of herringbone structures included in the whole 680 microstructure. Therefore, these specific microstructures do not store 681 any elastic energy and should not develop any cracks during the SPT 682 and cooling processes, assuming the microstructure transforms to the 683 t phase all at once. For finite aspect ratio, the obtained residual stress 684 are much smaller than those for all other microstructures. Interest-685 ingly, these microstructures are the ones expected in real t zirconia due 686 to the twinning plane being compatible with the crystal structures. 687

We aim to expand the present study to residual stress fields resulting 688 from the $t \to m$ SPT in pure zirconia. The *m* zirconia microstructures 689 are slightly more difficult to construct due to a larger number of variants 690 (namely 24) compared to the t case, but this should be very helpful to 691 interpret recent experimental data acquired with electron microscopy (Ors 692 et al., 2025) and with high resolution x-ray diffraction experiments at high 693 temperatures obtained on synchrotron beamlines (Guinebretière et al., 2022; 694 Purushottam Raj Purohit et al., 2022, 2024). 695

696 Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

700 Data availability

The data to reproduce these findings will be made available upon reasonable request.

703 Acknowledgment

This work was carried out within the framework of the HoTMiX research program funded by the agencies ANR (France) and DFG (Germany) under grant No. ANR-09-CE09-0035 and SCHM 997/37-1, respectively, as well as by the NanOX-ML program funded by ANR and FWF (Austria) under grant No. ANR-23-CE09-0041.

709 **References**

Aizu, K., 1970. Possible species of ferromagnetic, ferroelectric and ferroelas tic crystals. Phys. Rev. B 2, 754–772. doi:10.1103/physrevb.2.754.

Authier, A., 2003. International Table for Crystallography, vol. D: Physical Properties of Crystals. Kluwer Academic Publishers. doi:10.1107/
97809553602060000104.

- Backus, G.E., 1962. Long-wave elastic anisotropy produced by horizontal
 layering. J. Geophys. Res. 67, 4427–4440. doi:10.1029/jz067i011p04427.
- Boittin, G., Moulinec, H., Silva, F., 2024. CRaFT: composite response and
 Fourier transform. https://lma-software-craft.cnrs.fr/.
- Chiu, S.N., Stoyan, D., Kendall, W.S., Mecke, J., 2013. Stochastic Geometry
 and Its Applications. 3 ed., J. Wiley & Sons. doi:10.1002/9781118658222.
- Fadda, G., Truskinovsky, L., Zanzotto, G., 2002. Unified Landau description
 of the tetragonal, orthorhombic, and monoclinic phases of zirconia. Phys.
 Rev. B 66, 174107. doi:10.1103/PhysRevB.66.174107.
- Francfort, G.A., Murat, F., 1986. Homogenization and optimal bounds in
 linear elasticity. Arch. Rational Mech. Anal. 94, 307—334. doi:10.1007/
 BF00280908.
- Furat, O., Petrich, L., Finegan, D., Diercks, D., Usseglio-Viretta, F., Smith,
 K., Schmidt, V., 2021. Artificial generation of representative single Liion electrode particle architectures from microscopy data. npj Comput.
 Mater. 7, 105. doi:10.1038/s41524-021-00567-9.

Groeber, M., Ghosh, S., Uchic, M.D., Dimiduk, D.M., 2008. A framework for
automated analysis and simulation of 3D polycrystalline microstructures.
Part 2: synthetic structure generation. Acta Mater. 56, 1274–1287. doi:10.
1016/j.actamat.2007.11.040.

Gu, T., Castelnau, O., Forest, S., Hervé-Luanco, E., Lecouturier, F., Proudhon, H., Thilly, L., 2017. Multiscale modeling of the elastic behavior of architectured and nanostructured Cu–Nb composite wires. Int. J. Solids Struct. 121, 148–162. doi:10.1016/j.ijsolstr.2017.05.022.

Guinebretière, R., Ors, T., Michel, V., Thune, E., Huger, M., Arnaud, S.,
Blanc, N., Boudet, N., Castelnau, O., 2022. Coupling between elastic
strains and phase transition in dense pure zirconia polycrystals. Phys.
Rev. Mater. 6, 013602. doi:10.1103/PhysRevMaterials.6.013602.

Hayakawa, M., Kuntani, N., Oka, M., 1989. Structural study on the tetragonal to monoclinic transformation in arc-melted ZrO2-2mol.%Y2O3 – I.
experimental observations. Acta Metall. 37, 2223–2228. doi:10.1016/
0001-6160(89)90148-X.

Hayakawa, M., Tada, M., Okamoto, H., Oka, M., 1986. Structural study on the cubic to tetragonal transformation in arc-melted ZrO2-3mol.%Y2O3.
Trans. Japan Inst. Metals 27, 750–760. doi:10.2320/matertrans1960.27.
750.

Idiart, M., 2007. Nonlinear sequential laminates reproducing hollow sphere assemblages. C. R. - Mec. 335, 363–368. doi:10.1016/j.crme.2007.04.
003.

Kelly, P.M., Francis Rose, L.R., 2002. The martensitic transformation in
ceramics — its role in transformation toughening. Prog. Mater. Sci. 47,
463–557. doi:10.1016/S0079-6425(00)00005-0.

Kisi, E.H., Howard, C.J., 1998. Elastic constants of tetragonal zirconia
measured by a new powder diffraction technique. J. Am. Ceram. Soc.
81, 1682–1684. doi:10.1111/j.1151-2916.1998.tb02533.x.

Krogstad, J.A., Lepple, M., Gao, Y., Lipkin, D.M., Levi, C.G., 2011. Effect
 of yttria content on the zirconia unit cell parameters. J. Am. Ceram. Soc.
 94, 4548–4555. doi:10.1111/j.1551-2916.2011.04862.x.

Landau, L.D., Lifshitz, E.M., 2013. Statistical Physics. 3 ed., Elsevier.
 doi:10.1016/B978-0-08-057046-4.50021-X.

Lang, S.M., 1964. Axial thermal expansion of tetragonal ZrO, between 1150°
and 1700° C. J. Am. Ceram. Soc. 47, 641–644. doi:10.1111/j.1151-2916.
1964.tb13125.x.

Lebensohn, R.A., Ponte Castañeda, P., Brenner, R., Castelnau, O., 2011.
Full-field vs. homogenization methods to predict microstructure-property
relations for polycrystalline materials, in: Ghosh, S., Dimiduk, D.
(Eds.), Computational Methods for Microstructure-Property Relationships. Springer, pp. 393–441. doi:10.1007/978-1-4419-0643-4_11.

Mamivand, M., Asle Zaeem, M., El Kadiri, H., Chen, L.Q., 2013. Phase field
modeling of the tetragonal-to-monoclinic phase transformation in zirconia.
Acta Mater. 61, 5223–5235. doi:10.1016/j.actamat.2013.05.015.

Milton, G.W., 2002. The Theory of Composites. Cambridge University
 Press. doi:10.1017/cbo9780511613357.

Moulinec, H., Suquet, P., 1998. A numerical method for computing
the overall response of nonlinear composites with complex microstructure. Comput. Methods Appl. Mech. Engrg. 157, 69–94. doi:10.1016/
S0045-7825(97)00218-1.

Ors, I., Gey, N., Huger, M., Castelnau, O., Guinebretière, R., 2025. Strains,
stresses and microcracks in pure zirconia polycrystals. Mater. Charact.
220, 114667. doi:10.1016/j.matchar.2024.114667.

Ors, T., Gouraud, F., Michel, V., Huger, M., Gey, N., Micha, J.S., Castelnau, O., Guinebretière, R., 2021. Huge local elastic strains in bulk nanostructured pure zirconia materials. Mater. Sci. Eng.: A 806, 140817.
doi:10.1016/j.msea.2021.140817.

Paux, J., Morin, L., Gélébart, L., Amadou Sanoko, A.M., 2025. A discrete
sine-cosine based method for the elasticity of heterogeneous materials with
arbitrary boundary conditions. Comput. Methods Appl. Mech. Eng. 433.
doi:10.1016/j.cma.2024.117488.

Plancher, E., Favier, V., Maurice, C., Bosso, E., Rupin, N., Stodolna, J.,
Loisnard, D., Marijon, J.B., Petit, J., Micha, J.S., Robach, O., Castelnau,
O., 2017. Direct measurement of local constitutive relations, at the micrometre scale, in bulk metallic alloys. J. Appl. Crystallogr. 50, 940–948.
doi:10.1107/S1600576717006185.

Purushottam Raj Purohit, R.R.P., Fowan, D., Arnaud, S., Blanc, N., Micha,
J.S., Guinebretière, R., Castelnau, O., 2024. Laue microdiffraction on
polycrystalline samples above 1500K achieved with the QMAX-μLaue furnace. J. Appl. Crystallogr. 57, 470–480. doi:10.1107/S1600576724001821.
Purushottam Raj Purohit, R.R.P., Fowan, D.P., Thune, E., Arnaud, S.,

⁸⁰² Furthshottam Raj Furonit, R.R.F., Fowan, D.F., Thune, E., Afnaud, S.,
⁸⁰³ Chahine, G., Blanc, N., Castelnau, O., Guinebretière, R., 2022. Phase
⁸⁰⁴ transition and twinning in polycrystals probed by in situ high temperature
⁸⁰⁵ 3D reciprocal space mapping. Appl. Phys. Lett. 121, 181901. doi:10.1063/
⁸⁰⁶ 5.0109058.

Purushottam Raj Purohit, R.R.P., Richeton, T., Berbenni, S., Germain, L., Gey, N., Connolley, T., Castelnau, O., 2021. 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 Mater. 208, 116762. doi:10.1016/j.actamat. 2021.116762.

Quey, R., Renversade, L., 2018. Optimal polyhedral description of 3D
polycrystals: method and application to statistical and synchrotron Xray diffraction data. Comput. Methods Appl. Mech. Eng. 330, 308–333.
doi:10.1016/j.cma.2017.10.029.

Redenbach, C., Liebscher, A., 2015. Random tessellations and their application to the modelling of cellular materials, in: Schmidt, V. (Ed.),
Stochastic Geometry, Spatial Statistics and Random Fields: Models and
Algorithms. Springer, pp. 73–93. doi:10.1007/978-3-319-10064-7_3.

Seitl, F., Petrich, L., Staněk, J., Krill III, C.E., Schmidt, V., Beneš, V.,
2020. Exploration of Gibbs-Laguerre tessellations for three-dimensional
stochastic modeling. Methodol. Comput. Appl. Probab. 23, 669–693.
doi:10.1007/s11009-019-09757-x.

Serrao, P.H., Sandfeld, S., Prakash, A., 2021. OptiMic: A tool to generate
 optimized polycrystalline microstructures for materials simulations. SoftwareX 15, 100708. doi:10.1016/j.softx.2021.100708.

Simha, N., 1997. Twin and habit plane microstructures due to the tetragonal
to monoclinic transformation of zirconia. J. Mech. Phys. Solids 45, 261–
292. doi:10.1016/S0022-5096(96)00074-9.

Smirnov, M., Mirgorodsky, A., Guinebretière, R., 2003. Phenomenological
 theory of lattice dynamics and polymorphism of ZrO₂. Phys. Rev. B 68,
 104106. doi:10.1103/PhysRevB.68.104106.

Suquet, P., Moulinec, H., Castelnau, O., Montagnat, M., Lahellec, N., Grennerat, F., Duval, P., Brenner, R., 2012. Multiscale modeling of the mechanical behavior of polycrystalline ice under transient creep, in: Cazacu, O. (Ed.), IUTAM Symp. Linking Scales in Computations: From Microstructure to Macro-scale Properties, pp. 76–90. doi:10.1016/j.piutam.2012.
03.006.

Wang, Y., Wang, H.Y., Chen, L.Q., Khachaturyan, A.G., 1995. Microstructural development of coherent tetragonal precipitates in magnesiumpartially-stabilized zirconia: a computer simulation. J. Am. Ceram. Soc.
78, 657–661. doi:10.1111/j.1151-2916.1995.tb08228.x.

Yashima, M., Ishizawa, N., Yoshimura, M., 1993. High-temperature Xray study of the cubic-tetragonal diffusionless phase transition in the
ZrO2-ErO1.5 system: I, phase change between two forms of a tetragonal phase, t'-ZrO2 and t"-ZrO2, in the compositionally homogeneous 14 mol% ErO1.5-ZrO2. J. Am. Ceram. Soc. 76, 641–648. doi:10.1111/j.
1151-2916.1993.tb03654.x.

Zhao, X.S., Shang, S.L., Liu, Z.K., Shen, J.Y., 2011. Elastic properties of
cubic, tetragonal and monoclinic ZrO2 from first-principles calculations.
J. Nucl. Mater. 415, 13–17. doi:10.1016/j.jnucmat.2011.05.016.

⁸⁵³ Appendix A. Exact results for a rank-2 thermo-elastic laminate

In this section, we recall the expression for the effective behavior of a rank-*n* thermo-elastic laminate (Milton, 2002) and we provide compact expressions for the residual stress field. Schematic representation of the microstructure of rank-1 and rank-2 laminates are shown in Figure 7.

In the rank-1 laminate, the unit vector normal to the layers is denoted **n**. These layers are denoted 'mechanical phases' in the following. Each layer has a different elastic stiffness **C** and stress-free strain ε^0 . The effective stiffness and effective stress-free strain of such a composite are denoted $\tilde{\mathbf{C}}$ and $\tilde{\varepsilon}^0$ respectively.

In a rank-2 laminate, each layer is itself a rank-1 laminate, and **n** now denotes the unit normal to the planar boundary between each of these rank-1 laminates. The stiffness and stress-free strain of each layer of the rank-2 laminate are thus those computed for the constituting rank-1 laminates. Solving for a rank-*n* laminate can thus be done iteratively.

The mechanical phases constituting the laminate are supposed to exhibit a thermo-elastic behavior

$$\boldsymbol{\varepsilon}(\mathbf{x}) = \mathbf{S}^{(r)} : \boldsymbol{\sigma}(\mathbf{x}) + \boldsymbol{\varepsilon}^{0(r)}, \qquad \boldsymbol{\sigma}(\mathbf{x}) = \mathbf{C}^{(r)} : \left(\boldsymbol{\varepsilon}(\mathbf{x}) - \boldsymbol{\varepsilon}^{0(r)}\right)$$
(A.1)

with $\mathbf{C}^{(r)}$ and $\mathbf{S}^{(r)}$ the elastic stiffness and compliance tensors, respectively, 870 and $\varepsilon^{0(r)}$ the stress-free (or thermal) strain, for the phase designed by its 871 index (r). Furthermore, $\sigma(\mathbf{x})$ is the stress tensor at position \mathbf{x} within the 872 laminate, while $\varepsilon(\mathbf{x})$ is the *total* strain tensor at \mathbf{x} , i.e. $\varepsilon(\mathbf{x})$ is the sum of the 873 elastic and stress-free deformations. Here, we use the notation $\chi^{(r)}$ when the 874 field $\chi(\mathbf{x})$ is uniform within phase r, i.e. when $\chi(\mathbf{x}) = \chi^{(r)}$ for all locations 875 \mathbf{x} in the phase (r). When the stress-free strain is due to thermal dilation, it 876 holds 877

$$\boldsymbol{\varepsilon}^{0\left(r\right)} = \boldsymbol{\alpha}^{\left(r\right)} \Delta T \tag{A.2}$$

with $\boldsymbol{\alpha}^{(r)}$ the local dilation modulus of phase (r) and ΔT the temperature change, supposed homogeneous within the laminate. We consider hereafter the case of general anisotropy for both the elastic stiffness and thermal strain (or dilation tensor). The elastic strain field is given by

$$\boldsymbol{\varepsilon}^{e}(\mathbf{x}) = \mathbf{S}^{(r)} : \boldsymbol{\sigma}(\mathbf{x}) \tag{A.3}$$

and is due to both the elastic accommodation of the incompatible thermal
strain and to elastic strain due to the applied macroscopic stress. The effective behavior is given by

$$\bar{\boldsymbol{\varepsilon}} = \tilde{\mathbf{S}} : \bar{\boldsymbol{\sigma}} + \tilde{\boldsymbol{\varepsilon}}^0 \tag{A.4}$$

with $\tilde{\mathbf{S}}$ the effective compliance and $\tilde{\boldsymbol{\varepsilon}}^0$ the effective thermal strain. One defines for a purely elastic problem (i.e. for which $\boldsymbol{\varepsilon}^{0(r)} = \mathbf{0}$ for all (r), e.g. when $\Delta T = 0$) the stress concentration tensor **B** relating local and effective stresses

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbf{B}(\mathbf{x}) : \bar{\boldsymbol{\sigma}} \tag{A.5}$$

so that, for the thermo-elastic problem, the local stress can be expressed as

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbf{B}(\mathbf{x}) : \bar{\boldsymbol{\sigma}} + \boldsymbol{\sigma}^{res}(\mathbf{x})$$
(A.6)

with σ^{res} the field of residual stress. One can similarly define a strain localization tensor **A** such that, for a purely elastic problem,

$$\boldsymbol{\varepsilon}(\mathbf{x}) = \boldsymbol{\varepsilon}^e(\mathbf{x}) = \mathbf{A}(\mathbf{x}) : \bar{\boldsymbol{\varepsilon}} .$$
 (A.7)

⁸⁹² It is thus true that, for any microstructure,

$$\tilde{\mathbf{C}} = \langle \mathbf{C} : \mathbf{A} \rangle , \quad \tilde{\mathbf{S}} = \langle \mathbf{S} : \mathbf{B} \rangle , \quad \tilde{\varepsilon}^0 = \langle \varepsilon^0 : \mathbf{B} \rangle , \quad (A.8)$$

together with $\langle \mathbf{A} \rangle = \langle \mathbf{B} \rangle = \mathbf{I}$ where $\langle . \rangle$ denotes the volume average over the whole laminate volume.

Accounting for their specific microstructure, the effective elastic stiffness $\tilde{\mathbf{C}}$ for rank-1 laminates is given by the following *exact* expression (Milton, 2002)

$$\left[C_0(C_0\mathbf{I} - \tilde{\mathbf{C}})^{-1} - \mathbf{\Gamma}^1(\mathbf{n})\right]^{-1} = < \left[C_0(C_0\mathbf{I} - \mathbf{C}^{(r)})^{-1} - \mathbf{\Gamma}^1(\mathbf{n})\right]^{-1} > (A.9)$$

with C_0 an arbitrary stiffness used to introduce the polarization field and **I** the fourth order identity tensor with components $I_{ijkl} = \frac{1}{2}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$. The projection tensor Γ^1 only depends on the unit normal **n**

$$\Gamma^{1}_{ijlm} = \frac{1}{2} (n_i \delta_{jl} n_m + n_i \delta_{jm} n_l + n_j \delta_{il} n_m + n_j \delta_{im} n_l) - n_i n_j n_l n_m \quad (A.10)$$

and the complementary tensor Γ^2 is defined as

$$\Gamma^1 + \Gamma^2 = \mathbf{I} \,. \tag{A.11}$$

A well-known remarkable result is that, for homogeneous boundary conditions, the stress and strain in laminates are *uniform* within each layer, i.e.

$$\boldsymbol{\sigma}(\mathbf{x}) = \boldsymbol{\sigma}^{(r)} , \ \boldsymbol{\varepsilon}(\mathbf{x}) = \boldsymbol{\varepsilon}^{(r)}$$
(A.12)

for all locations **x** within the phase (r) with some components being equal to their effective counterparts. This can be expressed as

$$\Gamma_1: \boldsymbol{\sigma}(\mathbf{x}) = \Gamma_1: \bar{\boldsymbol{\sigma}}, \text{ and } \Gamma_2: \boldsymbol{\varepsilon}(\mathbf{x}) = \Gamma_2: \bar{\boldsymbol{\varepsilon}}$$
 (A.13)

for all locations **x**. Considering the purely elastic problem, remarking that the local constitutive relation can be written $(\Gamma^1 + \Gamma^2)$: $\sigma = \mathbf{C}$: $(\Gamma^1 + \Gamma^2)$ Γ^2 : ε , and using the properties indicated above, it can be shown that the stress concentration tensor (which is uniform within phases) is given by the following expression

$$\mathbf{B}^{(r)} = \left[\mathbf{\Gamma}^1 : \mathbf{S}^{(r)} - \mathbf{S}^{(r)} : \mathbf{\Gamma}^2\right]^{-1} : \left[\mathbf{S}^{(r)} : \mathbf{\Gamma}^1 - \mathbf{\Gamma}^2 : \tilde{\mathbf{S}}\right]$$
(A.14)

⁹¹¹ and the strain localization by

$$\mathbf{A}^{(r)} = \left[\mathbf{\Gamma}^2 : \mathbf{C}^{(r)} - \mathbf{C}^{(r)} : \mathbf{\Gamma}^1\right]^{-1} : \left[\mathbf{C}^{(r)} : \mathbf{\Gamma}^2 - \mathbf{\Gamma}^1 : \tilde{\mathbf{C}}\right] .$$
(A.15)

To express the residual stress field, which turns out to be uniform in each phase, one has to remark that (A.13) combined with (A.11) leads to

$$\boldsymbol{\sigma} = \bar{\boldsymbol{\sigma}} + \boldsymbol{\Gamma}^2 : (\boldsymbol{\sigma} - \bar{\boldsymbol{\sigma}}), \qquad \boldsymbol{\varepsilon} = \bar{\boldsymbol{\varepsilon}} + \boldsymbol{\Gamma}^1 : (\boldsymbol{\varepsilon} - \bar{\boldsymbol{\varepsilon}}).$$
(A.16)

These latter expressions can be plugged into the local behavior $(A.1)_2$ to give

$$\left(\mathbf{S}^{(r)}:\mathbf{\Gamma}^2-\mathbf{\Gamma}^1:\mathbf{S}^{(r)}\right):\boldsymbol{\sigma}^{(r)}=\mathbf{\Gamma}^2:(\bar{\boldsymbol{\varepsilon}}-\boldsymbol{\varepsilon}^{0\,(r)})-\mathbf{S}^{(r)}:\mathbf{\Gamma}^1:\bar{\boldsymbol{\sigma}}.$$
 (A.17)

The residual stress is defined as the field of stress remaining in the material when there is no applied stress, i.e. for $\bar{\sigma} = 0$ leading also to $\bar{\varepsilon} = \tilde{\varepsilon}^0$. One thus gets

$$\boldsymbol{\sigma}^{res(r)} = \left(\mathbf{S}^{(r)}: \boldsymbol{\Gamma}^2 - \boldsymbol{\Gamma}^1: \mathbf{S}^{(r)}\right)^{-1}: \boldsymbol{\Gamma}^2: \left(\tilde{\boldsymbol{\varepsilon}}^0 - \boldsymbol{\varepsilon}^{0\,(r)}\right) \tag{A.18}$$

919 with $\tilde{\boldsymbol{\varepsilon}}^0$ given by (A.8).