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ESTIMATING STRESS FLUCTUATIONS IN POLYCRYSTALS USING AN IMPROVED MAXIMUM ENTROPY METHOD

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Abstract. The prediction of local field statistics from effective properties is an open problem in the field of micromechanics. Partial information on the local field statistics is accessible from homogenization assumptions. In particular, exact phase-wise second moments of stresses can be calculated analytically from the effective strain energy density. In recent years, full-field calculations have become efficient enough to sample large ensembles of microstructures in the plastic regime (e.g. Gehrig et. al [4]).

In the present work, the maximum entropy method known from statistical thermodynamics is used to estimate first and second moments of local stresses from known eigenstrain distributions. The simple and refined formulations of the maximum entropy method proposed by Kreher and Pompe [9] are considered. While the simple method yields satisfactory results for a large amount of material classes (cf. Krause and Böhlke [7]), we prove that it does not respect the linearity of the eigenstrain problem. We further show that neither method corresponds to the exact second moments of stresses known from the effective strain energy density. By incorporating additional information, we find an improved maximum entropy method.

As an example, we analyze stress fluctuations in polycristalline titanium. For the exact analytical solution and the maximum entropy methods, we use the singular approximation and the Hashin-Shtrikman bounds. For comparison, we numerically approximate full-field statistics using an FFT approach. In all methods, the stress fluctuations caused by the anisotropy of the single crystal strongly influence the elastic-plastic transition.

1 SIMPLE MEM FOR POLYCRYSTALS

1.1 General Principle

The maximum entropy method (MEM) relies on Shannon's information entropy, which can be thought of as representing the possible information content of a set of discrete states. In the context of statistical physics, Jaynes [5] extended the information entropy to continuous probability distributions. For a probability distribution p of a vector of random variables x, the amount of information is calculated using the information entropy functional

$$S = -\int_V p(x)\ln(p(x))\,\mathrm{d}x \tag{1}$$

where the integration volume V is the entire domain of p. Maximizing the information entropy maximizes the amount of information that is left to chance, which is equivalent to making no implicit assumptions about the structure of the considered problem. Any assumptions that ought to be made can be implemented into the entropy maximization problem as additional constraints.

In affine linear continuum micromechanics, the quantities of interest are the Cauchy stress $\boldsymbol{\sigma}$ and the total strain $\boldsymbol{\varepsilon}$. These are linked at every material point through the affine Hooke's Law using the stiffness tensor $\mathbb{C}$ and the thermal eigenstrain $\boldsymbol{\varepsilon}^{\theta}$ as material constants

$$\boldsymbol{\sigma} = \mathbb{C}[\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\theta}]. \tag{2}$$

The probability distribution of interest is the one-point joint probability distribution of local strains and material properties $p(\boldsymbol{\varepsilon}, \mathbb{C}, \boldsymbol{\varepsilon}^{\theta})$, as described by Kreher and Pompe [9]. The incidence probability of any given material property is assumed to be known, which is equivalent to prescribing a one-point probability distribution of material properties

$$p_1^{\mathrm{C}}(\mathbb{C}, \boldsymbol{\varepsilon}^{\theta}) = \int_{Sym} p(\boldsymbol{\varepsilon}, \mathbb{C}, \boldsymbol{\varepsilon}^{\theta}) \, \mathrm{d}\boldsymbol{\varepsilon}. \tag{3}$$

Effective (macroscopic) material properties and an effective load are prescribed using the effective affine Hooke's Law

$$\bar{\boldsymbol{\sigma}} = \bar{\mathbb{C}}[\bar{\boldsymbol{\varepsilon}} - \bar{\boldsymbol{\varepsilon}}^{\theta}]. \tag{4}$$

These effective quantities are defined using the ensemble average $\langle \cdot \rangle$, leading to additional constraints to the optimization problem

$$\bar{\boldsymbol{\varepsilon}} = \langle \boldsymbol{\varepsilon} \rangle, \quad \bar{\boldsymbol{\sigma}} = \langle \mathbb{C}[\boldsymbol{\varepsilon}] \rangle. \tag{5}$$

As the definition of effective material properties relies on the Hill-Mandel condition, that condition forms an additional optimization constraint

$$\langle \boldsymbol{\sigma} \cdot \boldsymbol{\varepsilon} \rangle = \langle \boldsymbol{\sigma} \rangle \cdot \langle \boldsymbol{\varepsilon} \rangle. \tag{6}$$

The Hill-Mandel condition holds for statistically homogeneous materials without pores or cracks as long as specific boundary conditions are prescribed, for example periodic boundary conditions. Then Equation 6 holds for any divergence-free field $\boldsymbol{\sigma}$ and any compatible field $\boldsymbol{\varepsilon}$, without requiring that the fields are connected by an elastic law. In a probabilistic single-point framework, ergodicity is not required, as shown by Kreher [9].

1.2 Application to thermoelastic polycrystals

The constrained optimization problem previously specified can be solved analytically using a Lagrange multiplier approach. By considering the elastic load and the thermal eigenstrains as separate problems, the local fields are split into mechanical and thermal contributions

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^{\mathrm{I}} + \boldsymbol{\varepsilon}^{\mathrm{II}}, \tag{7}$$

where the effective stress vanishes for the thermal contribution and the effective strain of the mechanical problem equals the macroscopically applied strain. From this definition, effective load constraints can be formulated for each of the split stress and strain fields. The Hill-Mandel condition similarly yields constraints for each combination of the split stress and strain fields. Each of these eight constraints $\boldsymbol{g}_i = 0$ as well as the function-valued material property constraint of Equation 3 is multiplied with a Lagrange multiplier λ of the corresponding dual vector space, leading to the modified optimization problem

$$\max_p S^*, \quad S^* = -\int_V p(\boldsymbol{\varepsilon}, \mathbb{C}, \boldsymbol{\varepsilon}^\theta) \ln(p(\boldsymbol{\varepsilon}, \mathbb{C}, \boldsymbol{\varepsilon}^\theta)) \, \mathrm{d}x + \sum_{i=1}^{9} \boldsymbol{g}_i \cdot \boldsymbol{\lambda}_i. \tag{8}$$

For single-phase thermoelastic polycrystals in particular, the local material properties depend only on the lattice orientation $\boldsymbol{Q}$. p_I^C can be defined in terms of the orientation distribution function (ODF) $f(\boldsymbol{Q})$.

Due to the ensemble averages, each constraint contains integrals, leading to a depiction of S^* as an integral over $p\ln(p)$ and constraint terms which are each linear in p. S^* is extremal when the partial derivative of the integrand by p is zero. This extremal point is a maximum according to Jaynes [6] and corresponds to

$$p(\boldsymbol{\varepsilon}, \boldsymbol{Q}) = \frac{f(\boldsymbol{Q})}{n} \exp\left(\sum_{\alpha=1}^{8} \frac{\partial \boldsymbol{f}_\alpha}{\partial p} \cdot \boldsymbol{\lambda}_\alpha\right), \tag{9}$$

where the functions $\boldsymbol{f}_\alpha$ are the interior parts of the ensemble averages within the constraints $\boldsymbol{g}_\alpha$ and n is a constant normalization parameter. After a bijective transformation of the Lagrange parameters, a Gaussian normal distribution emerges:

$$p(\boldsymbol{\varepsilon}, \boldsymbol{Q}) = f(\boldsymbol{Q}) \frac{1}{\sqrt{(2\pi)^6 \det(\mathbb{K})}} \exp\left(-\frac{1}{2}(\boldsymbol{\varepsilon} - \boldsymbol{\gamma}(\boldsymbol{Q})) \cdot \mathbb{K}^{-1}(\boldsymbol{Q})(\boldsymbol{\varepsilon} - \boldsymbol{\gamma}(\boldsymbol{Q}))\right). \tag{10}$$

The mean $\boldsymbol{\gamma}$ and the covariance $\mathbb{K}$ are dependent on the local lattice orientation and some macroscale constants. They can furthermore be specified separately for the I and II fields, including some coupling terms between both fields. Due to limited space in this publication, the interested reader is referred to Krause and Böhlke [7] for the full formulas.

1.3 Theoretical Inconsistencies

While the simple MEM derived above performs quite well, two theoretical inconsistencies are evident in the formulas. The first inconsistency disappears in Kreher's advanced MEM [8], while solving the other is the main goal of this work.

First, much of micromechanics assumes a particular linearity between effective and local fields. For the strain field, this is often expressed using strain localization tensors $\mathbb{A}$ and $\boldsymbol{a}$, defined such that

$$\boldsymbol{\varepsilon} = \mathbb{A}[\bar{\boldsymbol{\varepsilon}}] + \boldsymbol{a}. \tag{11}$$

While this notation is superficially similar to the split into I and II fields applied in the MEM, the two are not equivalent. It is generally assumed that $\boldsymbol{a}$ contains all thermal contributions to

the local strain, while $\mathbb{A}$ is caused solely by the stiffness contrasts of the material and therefore does not depend of $\boldsymbol{\varepsilon}^\theta$. By a coefficient comparison respective to $\bar{\boldsymbol{\varepsilon}}$, equivalent terms to $\mathbb{A}$ and $\boldsymbol{a}$ can be isolated from the MEM, where

$$\mathbb{A}_{\mathrm{MEM}} = \mathbb{A}^{\mathrm{I}} + \frac{1}{w_0}\boldsymbol{b}(\boldsymbol{\varepsilon}^\theta) \otimes \boldsymbol{c}(\boldsymbol{\varepsilon}^\theta), \tag{12}$$

$$\mathbb{A}^{\mathrm{I}} = \mathbb{C}^{-1}\mathbb{C}_-(\mathbb{C}_+ - \mathbb{C}_-)^{-1}(\mathbb{C}_+ - \bar{\mathbb{C}}) + (\mathbb{C}_+ - \mathbb{C}_-)^{-1}(\bar{\mathbb{C}} - \mathbb{C}_-), \tag{13}$$

$$\boldsymbol{b}(\boldsymbol{\varepsilon}^\theta) = (\boldsymbol{\varepsilon}^\theta + (\mathbb{C}_-^{-1} - \mathbb{C}_+^{-1})^{-1}[\boldsymbol{\varepsilon}_{\mathrm{s}} - \boldsymbol{\varepsilon}_{\mathrm{e}}] - (\mathbb{C}_+ - \mathbb{C}_-)^{-1}[\mathbb{C}_+[\boldsymbol{\varepsilon}_{\mathrm{s}}] - \mathbb{C}_-[\boldsymbol{\varepsilon}_{\mathrm{e}}]], \tag{14}$$

$$\boldsymbol{c}(\boldsymbol{\varepsilon}^\theta) = (\mathbb{C}_- - \bar{\mathbb{C}})(\mathbb{C}_+ - \mathbb{C}_-)^{-1}\mathbb{C}_+[\boldsymbol{\varepsilon}_{\mathrm{s}} - \bar{\boldsymbol{\varepsilon}}^{\mathrm{II}}]. \tag{15}$$

Along with the purely stiffness-dependent conventional term $\mathbb{A}^{\mathrm{I}}$, thermal terms appear which add an unexpected linear dependence of $\mathbb{A}$ on $\boldsymbol{\varepsilon}^\theta$. This inconsistency is addressed in section 2.1.

The second inconsistency arises in the covariance terms and must be treated separately from the first one. If no thermal eigenstrains are present, deriving the effective strain energy by the local stiffness yields the second statistical moment of strains

$$\frac{\partial \bar{w}}{\partial \mathbb{C}(\boldsymbol{Q})} = \frac{1}{2} f(\boldsymbol{Q}) \langle \boldsymbol{\varepsilon} \otimes \boldsymbol{\varepsilon} \rangle_{\boldsymbol{Q}}. \tag{16}$$

The MEM covariances yield a different result for the second statistical moment of strains:

$$\langle \boldsymbol{\varepsilon} \otimes \boldsymbol{\varepsilon} \rangle_{\boldsymbol{Q}} = \langle \boldsymbol{\varepsilon} \rangle_{\boldsymbol{Q}} \otimes \langle \boldsymbol{\varepsilon} \rangle_{\boldsymbol{Q}} + \mathbb{K}_{\mathrm{MEM}}. \tag{17}$$

In particular, the MEM covariance always has the same symmetry as local stiffness, which is not generally true for real microstructures, as the real microstructure covariance also depends on the direction of load. This inconsistency is addressed in section 2.2.

2 IMPROVED MEM FORMULATIONS

2.1 The Singular Approximation MEM

By incorporating the Eshelby assumption of ellipsoidal inclusions in a homogeneous reference matrix, the MEM can be formulated equivalently to the Singular Approximation. This is accomplished by initially considering the entropy of the infinite-point probability distribution of a displacement field $\boldsymbol{u}(\boldsymbol{x})$. In the immediate neighborhood of any given point, homogeneous properties are assumed, meaning that every point is within a spherical inclusion. A Green tensor is defined equivalently to other Eshelby-based approaches. If spatial correlations can be neglected, the non-singular part of the Green tensor vanishes, meaning that the Singular Approximation due to Fokin [3] is recovered in the MEM setting.

Instead of specifying the effective properties $\bar{\mathbb{C}}$, $\boldsymbol{\varepsilon}^\theta$ and $\bar{w}^{\mathrm{II}}$, this Singular Approximation Maximum Entropy Method (SA MEM) requires a reference stiffness $\mathbb{C}_0$ from which the effective properties can be calculated as in the Singular Approximation. With Eshelby's tensor $\mathbb{P}_0(\mathbb{C}_0)$, the effective stiffness can be written as by Walpole [14],

$$\tilde{\mathbb{C}}_0 = \mathbb{P}_0^{-1}(\mathbb{C}_0) - \mathbb{C}_0, \tag{18}$$

$$\bar{\mathbb{C}} = \langle (\mathbb{C} + \tilde{\mathbb{C}}_0)^{-1} \rangle^{-1} - \tilde{\mathbb{C}}_0. \tag{19}$$

To recapitulate, if $\mathbb{C}_0$ equals the zeroth-order bounds (cf. Nadeau and Ferrari [11]), the Hashin-Shtrikman-Bounds are recovered, while solving the nonlinear equation $\mathbb{C}_0 = \bar{\mathbb{C}}(\mathbb{C}_0)$ yields the self-consistent approximation.

The SA MEM yields means which are entirely consistent with the Singular Approximation means, in particular,

$$\mathbb{A} = (\mathbb{C} + \tilde{\mathbb{C}}_0)^{-1}(\bar{\mathbb{C}} + \tilde{\mathbb{C}}_0), \tag{20}$$

$$\boldsymbol{a} = (\mathbb{C} + \tilde{\mathbb{C}}_0)^{-1}(\tilde{\mathbb{C}}_0[\bar{\boldsymbol{\varepsilon}}^{\theta}] + \mathbb{C}[\boldsymbol{\varepsilon}^{\theta}]). \tag{21}$$

The SA MEM extends the Singular Approximation by approximating the covariances

$$\langle \mathbb{K} \rangle_{\boldsymbol{Q}} = \frac{1}{2}(d^{\mathrm{I}} + 2k + d^{\mathrm{II}})\mathbb{C}^{-1}(\mathbb{C} + \tilde{\mathbb{C}}_0)^{-1}\mathbb{P}_0^{-1}(\mathbb{C} + \tilde{\mathbb{C}}_0)^{-1}\mathbb{C}^{-1}. \tag{22}$$

2.2 Exact Phasewise Covariances

If the effective strain energy density is given as an expression of arbitrarily anisotropic phase stiffness tensors, phasewise second moments of strain can be recovered using a variational argument, assuming the Hill-Mandel condition holds. This relationship applies not only to polycrystals but also heterogeneous materials with discrete phases, such as inclusion-matrix composites, where with the phase index α,

$$\frac{\partial \bar{w}}{\partial \mathbb{C}_\alpha} = \frac{1}{2} c_\alpha \langle \boldsymbol{\varepsilon} \otimes \boldsymbol{\varepsilon} \rangle_\alpha. \tag{23}$$

To actually calculate this exact second moment, there exists the more practical effective stiffness form

$$\langle \boldsymbol{\varepsilon} \otimes \boldsymbol{\varepsilon} \rangle_\alpha = \frac{1}{c_\alpha} \left(\frac{\partial \bar{\mathbb{C}}}{\partial \mathbb{C}_\alpha} \right)^{\mathsf{T_H}} [\bar{\boldsymbol{\varepsilon}} \otimes \bar{\boldsymbol{\varepsilon}}], \tag{24}$$

which in the case of the Singular Approximation can be further specified as

$$\frac{\partial \bar{\mathbb{C}}}{\partial \mathbb{C}_\alpha} = \frac{\partial \bar{\mathbb{C}}}{\partial \mathbb{C}_0} \frac{\partial \mathbb{C}_0}{\partial \mathbb{C}_\alpha}. \tag{25}$$

The first term $\partial \bar{\mathbb{C}} / \partial \mathbb{C}_0$ can be calculated analytically, though to the authors' knowledge no clear derivation has been published yet. $\partial \mathbb{C}_0 / \partial \mathbb{C}_\alpha$ is a microstructure-specific parameter. This parameter generally has a lower bound due to the positive definiteness of the covariance, but no strict upper bound is known.

When $\partial \mathbb{C}_0 / \partial \mathbb{C}_\alpha$ is known, the phasewise second moments can be prescribed as an additional optimization constraint to the MEM. The result is a straightforward replacement of the MEM's usual elastic covariance by the prescribed value, resulting in

$$\begin{aligned} \mathbb{K}_\alpha = & \frac{1}{v_\alpha} \left(\frac{\partial \bar{\mathbb{C}}}{\partial \mathbb{C}_\alpha} \right)^{\mathsf{T_H}} \left[\bar{\boldsymbol{\varepsilon}}^{\mathrm{I}} \otimes \bar{\boldsymbol{\varepsilon}}^{\mathrm{I}} \right] - \langle \boldsymbol{\varepsilon}^{\mathrm{I}} \rangle_\alpha \otimes \langle \boldsymbol{\varepsilon}^{\mathrm{I}} \rangle_\alpha \\ & + (2k + d^{\mathrm{II}})\mathbb{C}^{-1}(\mathbb{C} + \tilde{\mathbb{C}}_0)^{-1}\mathbb{G}_0^{-1}(\mathbb{C} + \tilde{\mathbb{C}}_0)^{-1}\mathbb{C}^{-1}. \end{aligned} \tag{26}$$

Though the means and the elastic covariances are now given by the Singular Approximation, the MEM still provides additional knowledge in the form of the thermal strain covariances.

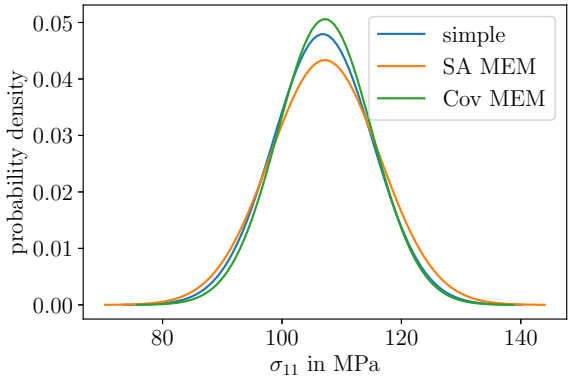

Figure 1: Probability density of σ_{11} in grains orthogonal to the loading direction (elastic)

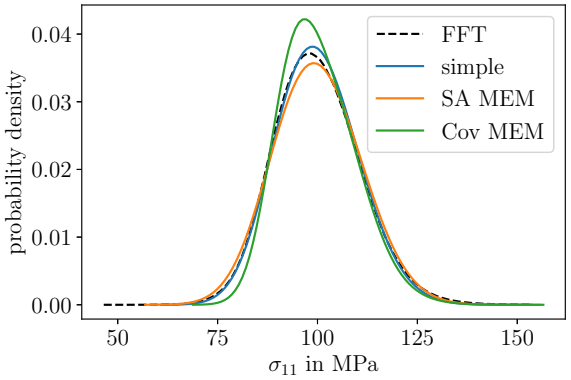

Figure 2: Overall probability density of σ_{11} for MEM approaches compared to FFT (elastic)

3 EXAMPLE: POLYCRYSTALLINE TITANIUM

As an illustrative example, polycrystalline titanium is considered. The ODF of the material is constant and the single crystals are spherical on average. The hexagonal single crystal stiffness measured by Dryburgh et al [2] is used. A unidirectional stress load of 100 MPa is applied.

Numerical full-field simulations are used for comparison. These are performed on a Laguerre tesselation microstructure with 8000 grains on 256^3 voxels using the Fast-Fourier-Transformation (FFT) approach pioneered by Moulinec and Suquet [10]. The implementation used here is based on the staggered grid discretization by Schneider et al [13], which reduces Gibbs oscillations.

The analytical approach is based on the Singular Approximation, where the reference stiffness is chosen as the Voigt stiffness. This results in an effective stiffness which lies inside the Hashin-Shtrikman bounds and deviates less than 0.5 % from the numerical stiffness obtained from the FFT simulations.

For grains oriented orthogonally to the loading direction, the probability distribution of stress is shown in Figure 1. As can be seen, all three MEM methods roughly agree on the mean and covariance. No reference full-field distribution is given because only a few grains of an appropriate orientation can be found in the present microstructure. The statistics of a small number of grains are influenced strongly by neighborhood effects and are therefore not representative for all grains of the same orientation. A large ensemble calculation averaging out these effects has been compared to the MEM by Gehrig et al. A preprint of that work is available at [4].

Overall probability distributions were calculated by integrating the MEM grain distributions over SO(3) with a Monte-Carlo approach. The results are shown in Figure 2 and compared to full-field results. As can be seen, the simple and SA MEM results are almost normally distributed, as are the full-field results. Based on these results, no clear recommendation of the simple or advanced MEM can be made. The improved MEM considering the exact covariances performs significantly worse, yielding a slightly skewed probability distribution. A possible explanation for this discrepancy lies in the reference stiffness derivative $\partial\mathbb{C}_0/\partial\mathbb{C}_\alpha$, which appears to be too dissimilar to the corresponding value in the FFT simulation. A homogenization approach which is well-chosen in regards to the effective stiffness parameter does not necessarily yield an accurate effective stiffness derivative. The sensitivity of the MEM to this additional parameter means that

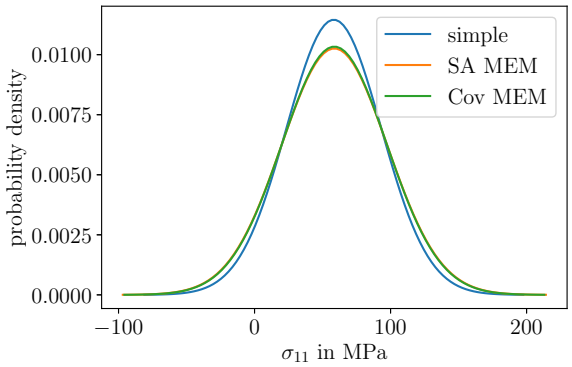

Figure 3: Probability density of σ_{11} in grains orthogonal to the loading direction (thermoelastic)

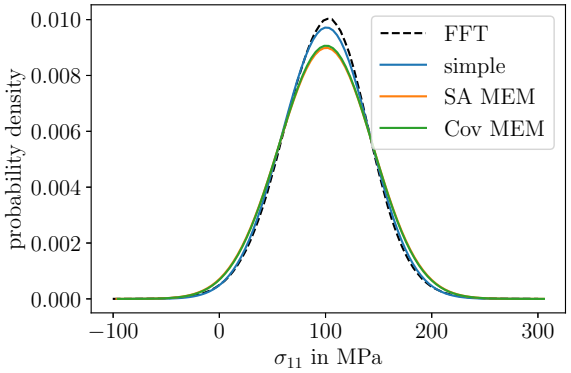

Figure 4: Overall probability density of σ_{11} for MEM compared to FFT (thermoelastic)

it can be used to describe microstructures which do not conform well to the simple or SA MEM approaches.

As an example for local stress fluctuations caused by eigenstrains, thermal eigenstrains were considered by using the anisotropic thermal expansion coefficients measured by Pawar and Deshpande [12]. An approximate guess for the reference temperature below which the local stress fluctuations start to develop during the cooling process is given by the stress relief treatment temperature of 480 °C given by Donachie [1].

For grains oriented orthogonally to the loading direction, the probability distribution of stress is given in Figure 3. The covariances are now substantially higher than in the purely mechanical case as thermal contributions dominate. The advanced and exact covariance methods therefore almost coincide. In the overall distributions given in Figure 4, it can be seen that the simple MEM approach again matches the FFT results most closely. The SA MEM, despite its theoretical soundness regarding the coupling of elastic and thermal terms, appears to perform worse in a context where this coupling becomes relevant. Again it should be noted that these results are true for a particular type of polycrystal microstructure. Kreher and Pompe [9] report better results with the SA MEM that the simple MEM for matrix-inclusion two-phase composites particularly as the elastic phase contrast increases.

4 CONCLUSIONS

Of the three variants of the MEM used to investigate titanium polycrystals, each is found to have different strengths and weaknesses. Kreher's simple MEM [9] performs particularly well for polycrystals with an isotropic orientation distribution function and roughly spherical grains. Its weaknesses lie in two theoretical shortcomings, a spurious dependence of the elastic localization on thermal quantities and a not generally expected proportionality of the covariance to the local stiffness.

The first shortcoming is solved in Kreher's advanced MEM [8] which is compatible to the Singular Approximation [3] and extends it by covariance terms. In the particular case considered here, the advanced MEM is less accurate than the simple MEM, particularly when thermal eigenstrains are considered. These results are not an indication of how these performance discrepancies

manifest in other use-cases such as matrix-inclusion microstructures.

The second shortcoming is solved by incorporating micromechanical exact covariance relations into the advanced MEM. Again, these improvements leads to larger differences to full-field results than the simple MEM approach in the case considered here. As the exact covariance relations introduce an additional microstructural parameter, a careful choice of this parameter might lead to more accurate results. The increased skew of the overall probability distributions suggest that this approach might be capable of modeling microstructures to which the simple MEM is not well-suited.

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