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Estimating Stress Fluctuations in Polycrystals with an Improved Maximum Entropy Method

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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. Kasemer et. al [1]).

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 [2] are considered. While the simple method yields satisfactory results for a large amount of material classes (cf. Krause and Böhlke [3]), 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.

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