Understanding stress and strain partitioning in polycrystalline materials using statistical machine learning

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How does a macroscopic applied stress or strain field distribute or partition into individual grains of a polycrystalline material? This is a long-standing question in the field of (poly)-crystal plasticity. The well-known Taylor and Sachs models provide bounds in this regard, with the Taylor model enforcing iso-strain – i.e., all grains obtain the same macroscopic applied strain – and the Sachs model enforcing iso-stress; the response of real materials lies somewhere in between.

In a recent work, we developed a methodology using statistical machine learning to understand strain partitioning in nanoscale polycrystalline thin films [1]. Such films constitute interesting material systems since they often display enhanced mechanical properties in comparison to their bulk counterparts. We perform atomistic simulations of the molecular statics/dynamics kind to understand the deformation mechanisms in thin film structures. Subsequently, we apply statistical machine learning algorithms to understand the inhomogeneity in the distribution of total strain, elastic strain and orientation in the structure. The results show a lognormal-like distribution of the elastic strain which is in contrast to the normal distribution observed for coarse-grained materials. Whilst the distribution of the elastic strain is unimodal, the distribution of total strain (and microrotation) is multimodal consisting of distinct peaks. We use a Gaussian mixture model to identify these peaks, and furthermore, correlate the individual peaks with deformation events occurring in individual grains.

We extend the methodology to analyze strain partitioning in crystal plasticity finite element simulations, and compare the results with those from atomistic simulations. Furthermore, we study the partitioning behavior over the entire trajectory of deformation. The results are finally discussed in the context of homogenization models and bridging length scales towards continuum frameworks.

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