Stresses at grain boundaries from FFT-based solvers

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In order to assess the question of brittle fracture within polycrystals, statistical approaches are proposed to derive failure probability laws from the combination of a statistical distribution of defects (such as inclusions) together with a statistical description of the heterogeneous stress field arising within the polycrystalline volume element when submitted to an average loading. Considering per grain average stresses distributions is suitable to deal with trans granular fracture [1] while dealing with inter-granular fracture requires the evaluation of Normal Stresses at Grain Boundaries (NSGB). Evaluating NSGB can be obtained with a standard Finite Element code using a mesh adapted to the polycrystalline geometry [2]. However, this approach may become prohibitive if both the number of grains or the mesh resolution, required to obtain converged results, becomes important. On the other hand, FFT-based solvers are much more efficient [3], and efficiently parallelized, but they rely on a regular mesh which does not coincide with the grain boundaries and seems inadequate to evaluate stresses at grain boundaries.

An important point of the presentation is to demonstrate that FFT-based solvers can be used to efficiently determine NSGB. For that purpose, a simple aggregate (27 voronoï cells) is considered and submitted to a uniaxial tensile loading together with periodic boundary conditions. The FE code [4] is used on a mesh adapted to the grain geometry and the NSGB is evaluated from an extrapolation of stresses at Gauss points in the connected elements. The FFT-based [5] solver is used on a regular mesh and the simulation can be performed with or without composite voxels (i.e. voxels crossed by a grain boundary) [6]. The comparison is performed on 'per grain boundary average normal stresses', in the context of linear elasticity (anisotropic), and non-linear crystal plasticity in both the infinitesimal and finite strains frameworks. After this comparison, results are statistically discussed on larger aggregates for different families of slip systems.

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