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## Which aggregate complexity is required for an accurate computation of stress and plastic strain fields?

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The increasing efficiency of computations allows the numerical evaluation of stress and plastic strain fields in aggregates which description is finer and finer. Either the FE method or the FFT method may be used. During the two last decades, such numerical computations lead to many new results, for instance allowing the validation of mean field homogenisation schemes. Nevertheless, some open questions remain such as:

- How detailed should the aggregate description be for allowing an accurate computation of the macroscopic behaviour, mean grain stress and plastic strain distributions, full fields?
- What is the effect of the neighbouring grains with respect to the orientation/shape of the considered grain itself?

Two homogenization approaches have been used for the sake of comparison:

- Two self-consistent mean-field approaches: the Kröner and the Hutchinson models;
- Crystalline finite element computations carried out on large aggregates. Various shapes of grains have been used: cube, Voronoï polyhedron or even more realistic grain shapes (Fig. 1). Either homogeneous grain size or measured grain size distributions have been considered. Finally, a 3D mesh containing 1370 surface and bulk grains has been built based on forty sequences including surface repolishing and EBSD measurements, carried out at Institut P' on a 316L austenitic stainless steel (Fig. 1 d). This very realistic aggregate contains a large number of annealing twins.

The cyclic elastic behaviour has been simulated first. In agreement with many experimental observations, crystals are separated into two orientation families [1,2]. The first family, located in the centre of the standard stereographic triangle (SST), gathers grains oriented for single slip which display generally persistent slip bands. That is why the activation of only one slip is allowed. The second family is located at the periphery of the SST and gathers grains oriented for multiple slip which exhibit labyrinths or cell/wall arrangements. As grain size effect is low in FCC metals of medium to high SFE, the crystal plasticity parameters are adjusted using experimental single crystal data only. Cubic elasticity is used.

The predicted macroscopic cyclic stress-strain curves are in fair agreement with experimental data for various loading conditions (tension-compression, shear, biaxial loading). The considered grain shape and grain size distribution affect only weakly the computed macroscopic behaviour. Surprisingly, the mean grain stress and plastic strain distributions depend only slightly on the details of the aggregate description (Figs. 1), in agreement with

previous 2D results [3]. But the full fields depend on these details because of stress / plastic strain concentrations close to grain boundaries and triple points.

Independently of the homogenisation model and constitutive laws, the computed distributions of mean grain plastic strain become narrower with increasing remote plastic strain. These results are in a qualitative agreement with many experimental observations showing that the dislocation microstructures become more homogeneous as the plastic strain increases [4]. On the contrary, the mean grain axial stress distributions become more scattered at high plastic strains, in agreement with the trends measured by X-ray diffraction [2].

The considered mean-field approaches neglect the effect of the neighbour grains. The deduced amplitudes of the mean grain distributions remain about two times lower than the one predicted by crystalline finite element calculations, whatever the remote plastic strain and the refinements in the microstructure description. This agrees with previous results concerning cubic elasticity only [5].

Finally, the effect of cubic elasticity and plasticity anisotropies is discussed. If multiple slip is allowed, the ratio between the saturated macroscopic tensile stress and the mean resolved shear stress is found to be about 2.6, in agreement with recent FFT computations assuming perfect plasticity [6]. The effect of hardening on the computed ratio value is very low. This value differs strongly from the well-known value of the Taylor factor, 3.06.

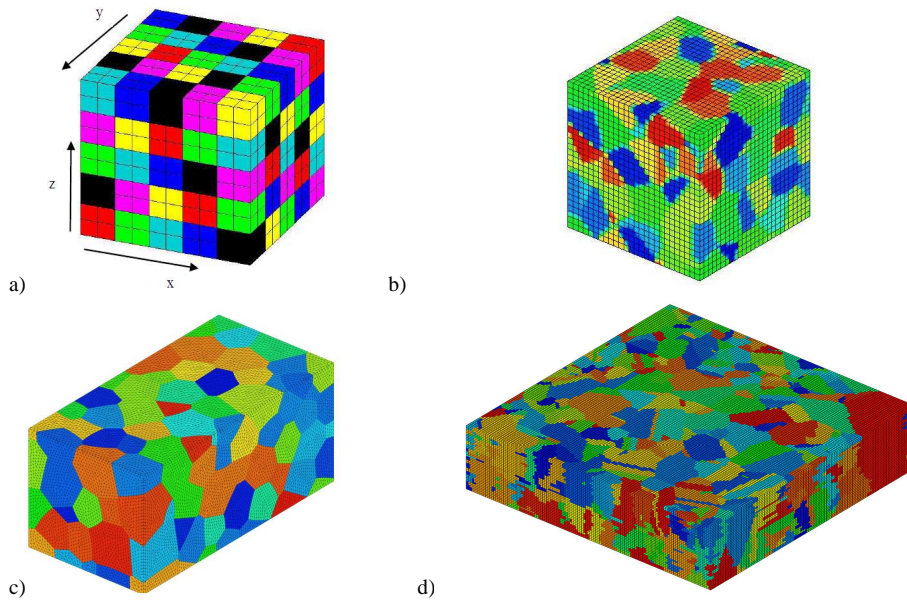


Figure 1: More and more realistic microstructures meshed using the FE software, Cast3M: (a) cubic grains, (b) polyhedra with staircase boundaries (c) modified Voronoi polyhedra and (d) reconstructed 3D aggregate based on repeated polishings and EBSD measurements.

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