An analysis of the influence of grain size on the strength of FCC polycrystals by means of computational homogenization

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ABSTRACT

It is well established that the flow stress and the hardening of polycrystalline materials depends on the grain size and various phenomenological laws (i.e. Hall-Petch) have been proposed based on experimental results or theoretical approximations [1]. There is not, however, a clear consensus on the physical micromechanisms underlying this effect. The development of dislocation pileups and formation of GND has been classically identified as the main mechanism responsible of this effect. However, depending on the initial dislocation density and grain size range other contributions such as the limitation of the dislocation mean free path near grain boundaries, may become crucial. In order to provide a deeper understanding, the influence of grain size on the mechanical response of FCC polycrystalline aggregates was analysed by means of computational homogenization. The mechanical response of each crystal follows a rate dependent physically based crystal plasticity model in the context of finite strain plasticity. In the model the critical resolved shear stress on each slip system is linked with the dislocation densities by a Taylor model [2]. The evolution of dislocation density in each slip system was governed by a Kocks–Mecking law in which the multiplication term, inversely proportional to the dislocation mean free-path, depends on the distance of the material point to the grain boundary. As much as possible, the model parameters were obtained from simulations at lower length scales, mainly dislocation dynamics simulations [2].

The constitutive model was implemented in Abaqus as a UMAT and the effect of grain size (in the range of 10 μm to 100 μm) on the mechanical response of a typical FCC metal (Al) was analysed by means of computational homogenization of a polycrystal [3]. A parametrical study was carried out to assess the influence of different microstructural parameters (grain size distribution, texture, initial dislocation density, etc.) on the effect of grain size on the flow stress and hardening of the material. These results were used to rationalize the different experimental results found in the literature and to ascertain the dominant factors that control that influence of the grain size effect in FCC polycrystalline metals.

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