Dislocation dynamics simulation of FCC single crystals in high strain rate deformation

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Résumé

In the range of high strain rate deformations from 10^{4} to 10^{6} s⁻¹ or more, the mobile dislocation density significantly increases and some dislocations may reach a large fraction of sound velocity. The extent of this mobile dislocation multiplication stage depends upon material, experimental or simulation conditions. It also strongly depends on the initial dislocation density. When the total dislocation density reaches a certain value, it may saturate [1].

Molecular dynamics simulations are well suited for very high strain rates (10^7 s⁻¹ or more). Hoverver, owing to the extremely small volumes and simulation times, it cannot deal with smaller strain rates. As a consequence, another type of simulation is needed for strain rates below 10^6 s⁻¹ and dislocation dynamics simulations appears to be the most suitable method for this purpose.

The first dislocation dynamics studies at high strain rates were performed in small volumes (2-5 microns) of copper single crystals [2-5]. The dislocation fluxes and artefacts such as self annihilations were not carefully handled [6]. In addition, plastic strains were quite small (less than 0.2%) for such volume sizes and the saturation of the mobile dislocation density was difficult to reach even for the lowest strain rate. Nevertheless, the effect of inertia above 10^3 s^{-1} [2] and, above all, the importance of cross-slip [3-5] were established.

With growing computing power, larger volumes and deformations can be reached and the end of the multiplication stage of high strain rate deformation can be reached. So this topic deserves being revisited. Results about dislocation velocities, mobile and total dislocation densities, as well as the anisotropic response of copper single crystal as a function of stain rate and the effect of cross-slip will be discussed. Références

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Mots-Clés: Dislocation dynamics, FCC single crystals, High strain rate deformation

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