Numerical prediction of the cyclic behaviour of metallic polycrystals and comparison with experimental data

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Abstract. Grain size seems to have only a minor influence on the cyclic strain curves (CSSCs) of metallic polycrystals of medium to high stacking fault energy (SFE). Many authors therefore tried to deduce the macroscopic CSSCs curves from the single crystals ones. Either crystals oriented for single slip or multiple slip were considered. In addition, a scale transition law should be used (from the grain scale to the macroscopic scale). The Sachs rule (homogeneous stress, single slip) or the Taylor one (homogeneous plastic strain, multiple slip) were usually used. But the predicted macroscopic CSSCs do not generally agree with the experimental data for metals and alloys, presenting various SFE values. In order to avoid the choice of a particular scale transition rule, many finite element (FE) computations are carried out using meshes of polycrystals including more than one hundred grains without texture. This allows the study of the influence of the crystalline constitutive laws on the macroscopic CSSCs. Activation of a secondary slip system in grains oriented for single slip is either allowed or hindered (slip planarity), which affects strongly the macroscopic CSSCs. The more planar the slip, the higher the predicted macroscopic stress amplitudes. If grains oriented for single slip obey slip planarity and two crystalline CSSCs are used (one for single slip grains and one for multiple slip grains), then the predicted macroscopic CSSCs agree well with experimental data provided the SFE is not too low (austenitic steel 316L, copper, nickel, aluminium).

1. Introduction
Following experimental investigations, the effect of grain size is weak in metallic materials such as nickel [1] and copper [2,3]. That is why it seems possible to deduce the macroscopic cyclic behaviour (polycrystal scale) from the single crystal one (grain scale). Several authors showed that the Sachs homogenization model [4], which assumes that single slip occurs in each grain homogeneously, leads to reasonable predictions in the case of copper for plastic strain amplitudes lower than a few $10^{-4}$ [5,3]. This is in agreement with many observations showing that only one slip system is activated per grain provided the macroscopic plastic strain is low enough [2,3]. But, Gorlier showed that the Sachs model leads to large underestimation of the macroscopic stress amplitude whatever the applied strain for the more planar austenitic stainless steel 316L [6]. The Taylor model gives more accurate predictions for low strain even if its assumptions are not true (homogeneous plastic strain tensor which generally requires the activation of five slip systems per grain [7])! In fact, it was shown later that both Sachs and Taylor models lead to underestimations of the stress amplitude for aluminium and nickel [8]. In order to avoid the choice of particular homogenization hypothesis, large scale polycrystalline finite element (FE) computations are carried out [9-11]. Each grain obeys particular crystalline elastic-plastic laws. The influence of two important slip mechanisms is studied for FCC metals at room temperature: single slip versus multiple slip cyclic hardening and slip planarity.
2. Crystalline constitutive laws and FE computations

Crystalline elasticity is used because of the cubic symmetry of the FCC structure. Twelve slip systems (\{111\}<110>) are considered in each grain. The macroscopic predictions are based on three kinds of crystalline cyclic hardening laws for better understanding which mechanisms are the most influent.

2.1. Crystalline plasticity laws adjusted on the CSSCs of single crystals oriented for single slip and allowing secondary slip

In copper [12] as in nickel [13-14], the CSSCs of crystals oriented for single slip are very close together because of their similar dislocation microstructures made of persistent slip bands. These orientations belong to a rather large domain of the standard crystallographic triangle (Fig. 1). During cycling at low plastic strain amplitudes, the corresponding crystals/grains are plastically activated because of their high Schmid factor values (close to 0.5, figure 1) whereas the ones oriented for multiple slip are still elastically deformed because of their low Schmid factor values. At low strain, the coefficients of the crystalline plastic hardening laws could therefore be adjusted using only the CSSCs of the well-oriented crystal (Schmid factor: 0.5). In addition, Laird and co-workers showed experimentally that the cyclic hardening of crystals is mainly due to cyclic increase of the kinematics stress (long range stress) whereas the isotropic stress (short range stress) is rather constant whatever experimentally that the cyclic hardening of crystals is mainly due to cyclic increase of the kinematics stress (long range stress) whereas the isotropic stress (short range stress) is rather constant whatever experimentally that the cyclic hardening of crystals is mainly due to cyclic increase of the kinematics stress (long range stress) whereas the isotropic stress (short range stress) is rather constant whatever. As it was shown a long time ago, crystals oriented for multiple slip, such as <100> or <111>, display stronger hardening than crystals oriented for single slip (plastic slip versus resolved shear stress curves). The case of nickel was extensively studied [13-14,16] as well as the one of copper. For these orientations, the dislocation microstructures are often made of labyrinths and cells/walls respectively, which differ from the persistent slip band microstructure usually observed for crystals oriented for single slip (figure 1). Therefore, taking into account the stronger cyclic hardening of the grains for which the loading direction is close to these crystallographic directions could lead to higher hardening at the polycrystal scale. Following the idea of Schwab and Holste [17], the grains are divided in several sets. Only two domains are used for the sake of simplicity. The standard crystallographic triangle is divided in two domains using a simple criterion. If the ratio between the secondary and primary resolved shear stresses, \(\tau_\text{sec}/\tau_\text{pri}\), is lower than a critical value, \(r_\text{crit}\), the grain is considered as being oriented for single slip (figure 2). If the ratio is higher, the grain is oriented for multiple slip. The critical ratio, \(r_\text{crit}\), should be higher than 0.94 (value of this ratio for a well-oriented single crystal which is known to be oriented for single slip) and lower than 1 (sides of the standard crystallographic triangle) (figure 1). Finally, two different couples of non-linear kinematics hardening coefficients, \((C_{\text{single}}, \alpha_{\text{single}})\) and \((C_{\text{multiple}}, \alpha_{\text{multiple}})\), should be adjusted using the single crystal CSS curves (figure 2).

2.2. Additional effect of hardening laws based the CSSCs of crystals oriented for multiple slip

As it was shown a long time ago, crystals oriented for multiple slip, such as <100> or <111>, display stronger hardening than crystals oriented for single slip (plastic slip versus resolved shear stress curves). The case of nickel was extensively studied [13-14,16] as well as the one of copper. For these orientations, the dislocation microstructures are often made of labyrinths and cells/walls respectively, which differ from the persistent slip band microstructure usually observed for crystals oriented for single slip (figure 1). Therefore, taking into account the stronger cyclic hardening of the grains for which the loading direction is close to these crystallographic directions could lead to higher hardening at the polycrystal scale. Following the idea of Schwab and Holste [17], the grains are divided in several sets. Only two domains are used for the sake of simplicity. The standard crystallographic triangle is divided in two domains using a simple criterion. If the ratio between the secondary and primary resolved shear stresses, \(\tau_\text{sec}/\tau_\text{pri}\), is lower than a critical value, \(r_\text{crit}\), the grain is considered as being oriented for single slip (figure 2). If the ratio is higher, the grain is oriented for multiple slip. The critical ratio, \(r_\text{crit}\), should be higher than 0.94 (value of this ratio for a well-oriented single crystal which is known to be oriented for single slip) and lower than 1 (sides of the standard crystallographic triangle) (figure 1). Finally, two different couples of non-linear kinematics hardening coefficients, \((C_{\text{single}}, \alpha_{\text{single}})\) and \((C_{\text{multiple}}, \alpha_{\text{multiple}})\), should be adjusted using the single crystal CSS curves (figure 2).

2.3. Effect of slip planarity imposed to grains oriented for single slip

As it was shown a long time ago, crystals oriented for multiple slip, such as <100> or <111>, display stronger hardening than crystals oriented for single slip (plastic slip versus resolved shear stress curves). The case of nickel was extensively studied [13-14,16] as well as the one of copper. For these orientations, the dislocation microstructures are often made of labyrinths and cells/walls respectively, which differ from the persistent slip band microstructure usually observed for crystals oriented for single slip (figure 1). Therefore, taking into account the stronger cyclic hardening of the grains for which the loading direction is close to these crystallographic directions could lead to higher hardening at the polycrystal scale. Following the idea of Schwab and Holste [17], the grains are divided in several sets. Only two domains are used for the sake of simplicity. The standard crystallographic triangle is divided in two domains using a simple criterion. If the ratio between the secondary and primary resolved shear stresses, \(\tau_\text{sec}/\tau_\text{pri}\), is lower than a critical value, \(r_\text{crit}\), the grain is considered as being oriented for single slip (figure 2). If the ratio is higher, the grain is oriented for multiple slip. The critical ratio, \(r_\text{crit}\), should be higher than 0.94 (value of this ratio for a well-oriented single crystal which is known to be oriented for single slip) and lower than 1 (sides of the standard crystallographic triangle) (figure 1). Finally, two different couples of non-linear kinematics hardening coefficients, \((C_{\text{single}}, \alpha_{\text{single}})\) and \((C_{\text{multiple}}, \alpha_{\text{multiple}})\), should be adjusted using the single crystal CSS curves (figure 2).

For the single slip oriented grains, the CSSC of the well-oriented crystal is used (Schmid factor: 0.5). For grains oriented for multiple slip, the <100> crystal curve is used because it has been published in the literature for all the metallic materials we study (aluminium, copper, nickel, 316L). The initial critical shear stress, \(\tau_{\text{cr}}\), is considered to be the same for all grains, whatever their orientations.

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and co-workers [12,15]. But a very high value of the latent hardening coefficient is chosen. Therefore, primary plastic slip induces a so high hardening on the secondary slip system that only single slip is predicted in both crystals and grains oriented for single slip. For grains oriented for multiple slip, weak self and latent isotropic hardening coefficients are used. The experimental single crystal CSS curves used for the adjustment of the crystalline plasticity laws have been published in the cited references (for example: Cu [3], Ni [13-14,16], 316L [6]).

Figure 1. Isovalues of the ratio between secondary and primary shear stresses plotted in the standard triangle (courtesy from Th. Kruml). Bold line: ratio equal to 0.94, (value for well-oriented crystal, black circle). Orientations with PSBs (red stars) or labyrinths/cells (blue diamonds) (nickel [13-14,16]).

Figure 2. Two domains of orientations corresponding to either single slip or multiple slip. Standard crystallographic triangle. Two different couples of non-linear kinematics hardening coefficients, \((C_{\text{single}}, \alpha_{\text{single}})\) and \((C_{\text{multiple}}, \alpha_{\text{multiple}})\), should be adjusted using the experimental single crystal CSS curves.

3. Comparison between predicted and experimental polycrystalline cyclic stress strain curves
Numerical homogeneization is applied using the FE method. Many details concerning the FE computations are given in [8,11] (FE code, boundary conditions, minimum number of grains and FEs, number of cycles required for getting cyclic saturation…). A typical mesh of 125 cubic grains is used.

3.1. Crystalline plasticity laws adjusted on the CSSCs of single crystals oriented for single slip and allowing secondary slip
The predicted CSSCs are generally close to the ones predicted by the Sachs model, whatever the considered metal or alloy [8,11]. This means that the macroscopic stress level is generally underestimated even if the plastic strain is in the 10^{-5} to 10^{-3} range (figures 3 and 4 for copper and 316L steel respectively, red curves with triangles). As no particular assumption is made concerning the homogeneization procedure, some physical hardening mechanisms occurring at the grain scale should have been neglected. As the hardening of grains oriented for multiple slip leads to a reduced increase of the predicted stress, the effect of slip planarity in grains oriented for single slip is now investigated.

3.2. Effect of slip planarity imposed to grains oriented for single slip
Hindering secondary slip in grains oriented for single slip leads to stronger macroscopic hardening whatever the applied macroscopic strain. The choice of the critical ratio value affects the predicted macroscopic stress only for axial plastic strain amplitude higher than about 10^{-3}. If the macroscopic
plastic strain is lower, using the minimum (0.94) or maximum value (1) leads to close predicted macroscopic CSS curves because the grains belonging to the multiple slip family are not plastically deformed at low plastic strain. Following figures 3 and 4, imposing slip planarity by hindering secondary slip leads to reasonable predictions whatever the material (copper, 316L, aluminium) for plastic strain smaller than $10^{-3}$. For higher amplitude, multiple slip in the corresponding grains should be taken into account in order to avoid too strong hardening due to slip planarity. Following figure 1, a value of the critical ratio, $r_{crit}$, close to 0.95 seems reasonable at least for nickel. If a higher value is used, many more grains/crystals displaying multiple slip dislocation microstructures such as labyrinths or walls would be in the single slip domain meaning that the partition is less accurate.

**Figure 3.** Predicted & experimental macroscopic CSS curves. Green symbols: experimental data. Red curve with triangles: basic model (well oriented grain (WO), secondary slip is allowed) (2.1 and 3.1). Red curve with circles: enhanced model (both single slip and multiple slip grains with $r_{crit}$=0.95, planar slip is imposed to well-oriented grains (2.2, 2.3 and 3.2). Copper.

**Figure 4.** Predicted & experimental macroscopic CSS curves. Green symbols: experimental data. Red curve with triangles: basic model (well oriented grain (WO), secondary slip is allowed) (2.1 and 3.1). Red curve with circles: enhanced model (both single slip and multiple slip grains with $r_{crit}$=0.95, planar slip is imposed to well-oriented grains (2.2, 2.3 and 3.2). 316L

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