# PREDICTION OF DEFORMATION TEXTURES IN ZIRCONIUM BASED ON A SIMPLIFIED MODELLING OF GRAIN INTERACTION

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**ABSTRACT** The goal of this study is to apply a "multisite" crystal plasticity model to the prediction of texture evolution in zirconium deformed at high temperature. The model under consideration is an extension of the elastic-viscoplastic "multisite model" proposed by Delannay et al. [2005] which has been adapted to account for a new type of grain interaction (Van Houtte et al. [2005]). Predictions of the model are compared to experimental data. Two forming processes are considered: sheet rolling (Lebensohn et al. [1994]) and the torsion of a cylindrical bar (Sanchez et al. [2001]).

**INTRODUCTION:** Hexagonal close-packed (hcp) crystals usually demonstrate larger anisotropy than cubic crystals. When zirconium is deformed at high temperature, elongation or contraction along the c-axis can only be achieved by dislocation slip along pyramidal slip systems ($\{10\bar{1}0\}<\bar{1}2\bar{1}0>$). However, pyramidal slip requires a much larger resolved shear stress than basal ($\{0001\}<2\bar{1}\bar{1}0>$) and prismatic slip ($\{10\bar{1}1\}<\bar{1}\bar{1}23>$). Instead of undergoing a uniform deformation (as predicted by the Taylor model), grains tend to deform heterogeneously, reducing the activity of pyramidal slip systems. This has been demonstrated based on texture predictions obtained either with a self-consistent approach (Lebensohn et al. [1994]) or with crystal plasticity based finite element model (CPFEM, see Delannay et al. [2005] and Van Houtte et al. [2002]).

The multisite model adopts a different strategy. It assumes (i) that the deformation of each grain is predominantly influenced by short-range interaction with adjacent grains, (ii) that local strains deviate from their macroscopic average according to specific "relaxation modes", and (iii) that the macroscopic strain is achieved on average by every pair of adjacent grains. The model bears some resemblance with the LAMEL model (Van Houtte et al. [2002]) that was originally proposed for cubic metals with cold rolling microstructures (i.e. flat grains). However, it has been observed (Delannay et al. [2005]) that the relaxation modes of the LAMEL model are not efficient in the case of hot rolled zirconium. Therefore, the relaxation modes used in the present paper do not assume that grain boundaries are aligned parallel to the rolling plane. Instead, we follow the ALAMEL procedure (Van Houtte et al. [2005]) according to which grains interact across

a planar interface that is not necessarily parallel to the rolling plane (grains are assumed equi-axed).

**PROCEDURES, RESULTS AND DISCUSSION:** Two polycrystalline plasticity models are compared: the Taylor model and the multisite model with relaxation modes of the ALAMEL type (Van Houtte et al. [2005]). Material parameters are consistent with previous studies on zirconium (Delannay et al. [2005] and Lebensohn et al. [1994]): typical strain rate $g_0$=0.01/s, strain rate sensitivity m= 0.13, crititcal resolved shear stresses are such that $\tau_c^{pyramidal} = 10\tau_c^{prismatic}$ and $\tau_c^{basal} = 1.5\tau_c^{prismatic}$.

**Rolling of zirconium sheet** The two polycrystalline plasticity models are used to predict a hot rolling texture in a zirconium alloy subjected to 63% thickness reduction. The numerical simulations start with an initially isotropic texture. Numerical results are compared to experimental measurements based on the <0002> pole figure. As shown on the experimental pole figure (Fig. 1a), rolling of the zirconium plate induces a preferential alignment of the c-axis within or close to the plane containing ND (normal direction of the plate) and TD (transverse direction of the plate). The two models (Fig. 1b and Fig. 1c) overestimate the strength of the deformation texture but the multisite model is closer to experimental result. The Taylor model predicts that some crystals have their c-axis close to the rolling direction (RD). This erroneous texture component can be attributed to the fact that the Taylor model overestimates the activity of pyramidal slip systems. Table 1 shows that, under the Taylor model, all slip modes present a similar activity (35% of the deformation is achieved by pyramidal slip). The multisite model allows a substitution of pyramidal slip by prismatic and basal slip. In consequence, the multisite model performs a more accurate texture prediction.

**Torsion of zirconium bar** The two polycrystalline plasticity models are then used to predict a torsion texture in a zirconium alloy. The texture has been measured on the surface where the shear strain is 138% (Fig. 2a). Again, both models (Fig. 2b and Fig. 2c) overestimate the strength of the deformation texture but the prediction of the multisite model is most accurate. According to Table 1, the Taylor predicts more pyramidal slip (29%) than the multisite model (12%).

**CONCLUSIONS:** The assumption of a uniformly deforming polycristal leads to reasonable texture predictions in cubic materials (Van Houtte et al. [2005]) but in the case of zirconium, it gives too much importance to the pyramidal slip mode. Hence, texture predictions are erroneous. The multisite model, with interactions of the ALAMEL type provides more accurate texture predictions.

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Table 1: Analysis of the distribution of slip activity among the various slip modes

| | | Accumulated slip | | |
|---|---|---|---|---|
| | | prismatic | basal | pyramidal |
| Rolling | Taylor model | 35% | 30% | 35% |
| | Multisite | 43% | 35% | 22% |
| Torsion | Taylor model | 41% | 30% | 29% |
| | Multisite | 49% | 39% | 12% |

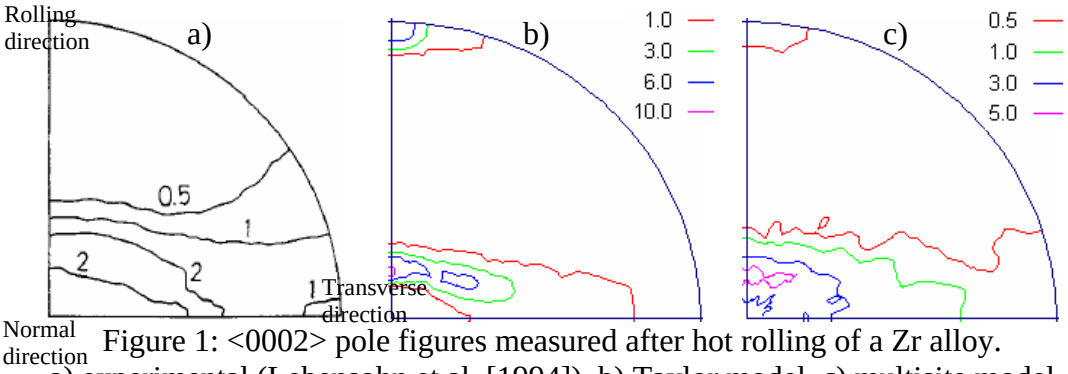


Figure 1: <0002> pole figures measured after hot rolling of a Zr alloy.
a) experimental (Lebensohn et al. [1994]), b) Taylor model, c) multisite model

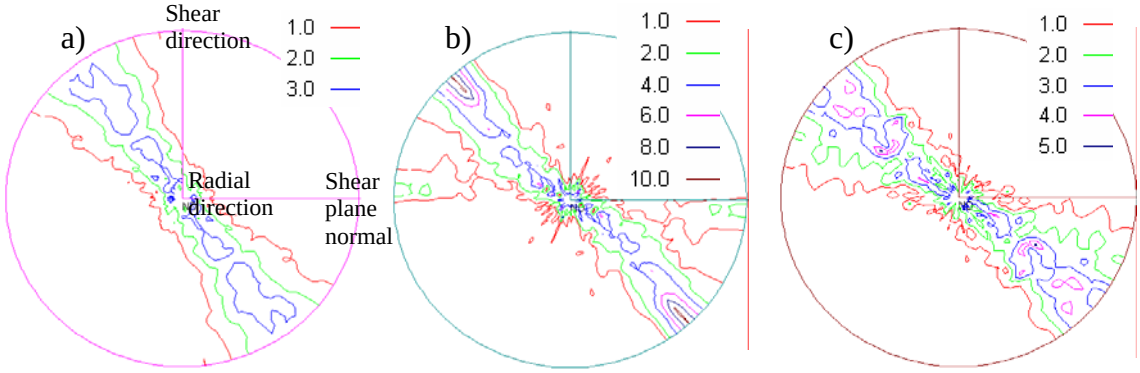


Figure 2: <0002> pole figures measured after torsion of a Zr alloy.
a) experimental (Sanchez et al. [2001]), b) Taylor model, c) multisite model

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