MODELING THE RELAXATION DUE TO TWINNING IN AN *HCP* ZIRCONIUM ALLOY

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Twinning can play an important part in the deformation of many metals, particularly those with lower crystal symmetries, for example zirconium, titanium, magnesium and their alloys. The twin is a region within a parent grain which has undergone a shear strain in response to stress characteristic of the particular twin system. This shear results in a crystallographic reorientation with respect to the parent crystal. As a consequence of this reorientation the physical properties of the twinned region (e.g. elastic constants) also have a different orientation from those of the parent grain. Further, this crystallographic re-orientation allows the accommodation of the deformation imposed on the parent grain by the stress, and hence results in a reduction in the stress in the parent grain.

Self-consistent models have been used extensively to simulate the elasto-plastic and visco-plastic deformation of anisotropic polycrystal materials, both for the prediction of deformation textures and to understand the contribution of various microscopic deformation modes to the macroscopic response. A new twinning model has recently been implemented within an Elasto-Plastic Self Consistent framework by Clausen and Tomé [1]. The model accounts for both crystallographic re-orientation and stress relaxation, and has provided improved agreement with experimental studies on the deformation of an extruded magnesium alloy [1]. Here, we compare the predictions of this new model against our extensive deformation neutron diffraction data set collected *in-situ* during deformation of Zircaloy-2 [2], a material which also undergoes twinning.

In addition, we have been carrying out a parametric finite element modeling study [3, 4] to investigate the possible stress states under which it is energetically favourable for twinning to occur, and the corresponding stress states after twinning both in parent grain and newly formed twin. The FE predictions are compared with the results obtained by fitting the EPSC model to the neutron diffraction data.

[1] Clausen, B., Tomé, C.N., Brown, D.W. & Agnew S.R., *in press* Acta Mater.
[2] Xu, F., Holt R.A., Daymond M.R., Rogge R.B. & Oliver E.C., *in press* Mat Sci Eng. A, doi:10.1016/j.msea.2007.11.018 (2007).
[3] Zhang, R.Y., Daymond, M.R. & Holt, R.A., Mat. Sci. Eng. A.; 473, p139-146 (2008).
[4] Zhang, R.Y., Daymond, M.R. & Holt, R.A., *to be submitted* Mat. Sci. Eng. A.