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# A methodology to obtain data at the slip-band scale from atomic force microscopy observations and crystal plasticity simulations.

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## *Abstract*

In this research article, a novel way to observe the micro-scale plastic deformation coupling atomic force microscopy and finite element calculation is introduced. The proposed methodology was also applied to study plastic strain localization quantitatively at the grain scale due to hydrogen embrittlement in the article.

***Keywords:*** atomic force microscopy, hydrogen embrittlement, finite element method, plastic deformation

Nowadays, crystal plasticity finite element method (CPFEM) is popular to be applied to solve the detailed deformation processes in metal materials. Compared to conventional finite element method, CPFEM is a more comprehensive way to model micro-level deformation, since it takes crystal information (grain orientation, grain size, dislocation/twinning slip directions and planes) into account. A recent paper published in *Acta Materialia* by I. Aubert, *et al*. introduced a new methodology to examine the grain-scale plastic deformation coupling atomic force microscopy and crystal plasticity finite element method. The effect of hydrogen in various kind of degradation in austenitic strainless steels is important, yet hard to be studied, since the effect could be masked by the geometrical and crystallographic heterogeneities in polycrystalline specimens. In this article, the authors proposed a novel way combining atomic force microscopy (AFM) measurements and crystal plasticity finite element simulation to trace the grain-level plastic deformation process, which can be an effective way to study hydrogen effect on the plastic strain localization.

Figure 1 briefly summarized this proposed methodology. As shown in this figure, after a specimen deformed, the surface topography was carefully measured using AFM. Based on the measured height of each slip step on the surface and the grain orientation, the total step height caused by dislocations in a given grain can be calculated. In the simulation part, the step heights caused by each of the all three slip systems can be respectively determined. Combined the two pieces of information, the total shear caused by dislocations (*i.e.* the plastic deformation within each grain) can be then calculated.

In the later part of this article, the authors applied this method to study the effect of absorbed hydrogen on emerging dislocations. The results clearly show that 70% of hydrogenated grains have both a higher number of dislocations per slip-band and a larger spacing between slip planes than hydrogen-free grains. Hydrogen effect on plastic localization at the grain scale is clearly evidenced and some hydrogenated grains exhibit a number of dislocation per slip-band up to 50 times higher and a spacing between slip planes 6 times larger than a hydrogen-free grain with the same plastic slip on the observed plane. This application is good evidence to prove the effectiveness of the proposed method.

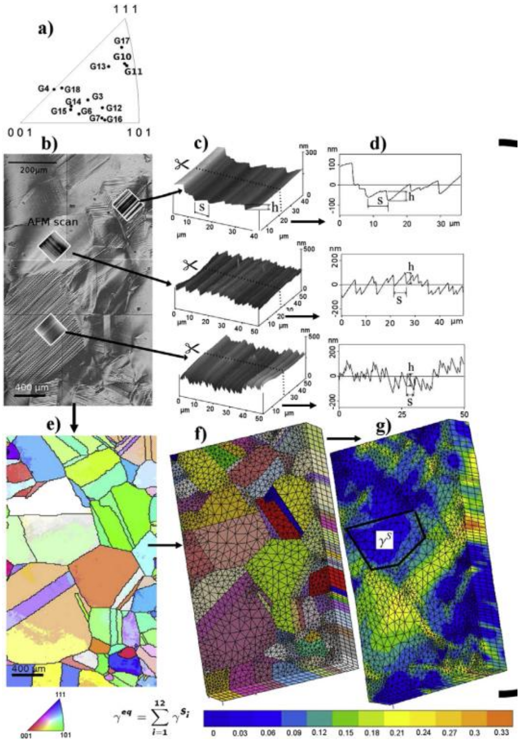

**Figure 1.** Methodology of the coupling AFM-observations and finite element results to obtain data at the slip-band scale. [1] (a) orientations, (b) SEM image and (e) EBSD map of the selected deformed grains; (c,d) AFM scan of the selected areas within the square boxes in (b); (f) mesh built for CPFEM; and (g) the total shear simulated by CPFEM.

This method has great potential to be highly automated with a careful design of software and hardware, which will provide a fast and effective way to measure local plastic deformation. In the future, the data measured using this presented approach is useful to study the relationship between plastic deformation localization and crack initiation.

## Reference

[1] I. Aubert, *et al.*, *Acta Mater.,* 2016, 104, pp. 9-17.