

In-Situ Bending and Structural Characterization of Penta-Twinned Silver Nanowires

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Metal nanowires are candidates for a variety of applications where their electric transport and optical properties offer possibilities for new technologies, for example flexible transparent and conductive films. As with all nanomaterials the extremely small size makes characterization of the materials challenging, making methods with extremely high spatial resolution, such as transmission electron microscopy (TEM) particularly important.

In this study samples of silver nanowires with the ‘penta-twinned’ nanostructure [1] were studied in the TEM. In this structure there are five symmetric twin planes within the nanowire all with a common [110] lattice direction along the wire axis. The wires were dispersed on a pre-prepared collodion film, that when irradiated by the electron beam would locally shrink, applying a compressive stress to the nanowires in the vicinity [2]. Under this compressive stress the wires were seen to bend elastically before failing through a highly localized bend with a seemingly abrupt interface (see the example in Figure 1a of a wire with a bend of approximately 38°)

This localized bend was then studied using scanning precession electron diffraction [3] in order to understand the local structural changes at ~1nm spatial resolution. A difficulty with this particular system is that the multiple twins in the structure mean that every diffraction pattern contains scattering from at least two of the five differently oriented crystals. To separate the individual diffraction signals the data was decomposed using non-negative matrix factorization [4] in the real space domain. From the decomposed data in the bent region of the wire it was possible to determine the overall orientation of the wire with respect to the beam direction (See Figure 1b) and hence the misorientation of the five twin-related segments of the nanowire across the deformation region (an example of the decomposed factor and loading for a twin-segment oriented close to [114] are shown in Figure 1c and 1d respectively).

The small size of each region in the nanowire reduced the likelihood of significant dislocation densities in the nanowire and the analysis indicated that the bend was entirely contained in-plane with no rotation around the common [110] direction, meaning the boundary is in fact a new twin in the majority of the segments of the wire. Studying the misorientations identified coincident site lattices (CSLs) [5] of type $\Sigma 7$ and $\Sigma 9$ between the upper and lower regions of the bent crystal segments, similar coincidence relations in other bent nanowires have also been determined by this analysis. Since CSLs offer some of the highest possible coordination between crystals, these should represent energetically favorable interface structures that wires can deform toward. The termination of this twin boundary at the wire surface was also seen to affect the geometry of the wire cross section with the region of the wire under tension becoming noticeably narrower while the region of the interface under compression becoming wider.

A general search through the major CSLs was performed to find those particular bending axis-angle conditions that could represent lower energy end-points for the bending process and these were used to

understand the distribution of bending angles measured from several hundred bent nanowires.

References:

- [1] Sun, M., Cao, R., Xiao, F. & Deng, C. *Comput. Mater. Sci.* **79**, (2013) p289–295.
- [2] Zheng, K. et al. *Nat. Commun.* **1**, (2010) p1–8.
- [3] Rauch, E. F., Véron, M., Portillo, J., Bultreys, D., Maniette, Y. and Nicolopoulos, S. *Microscopy and Analysis*, **22**(6), (2008) S5–S8
- [4] Lee, D. D. and Seung, H. S. *Nature*, **401** (1999) p 6755.
- [5] Grimmer, H., Bollmann, W. and Warrington, D. H. *Acta Crystallogr. A* **30**, (1974) p. 197–207.
- [6] The authors acknowledge funding from the Royal Society, the China Scholarship Council and the UK EPSRC through grant number EP/S009493/1.

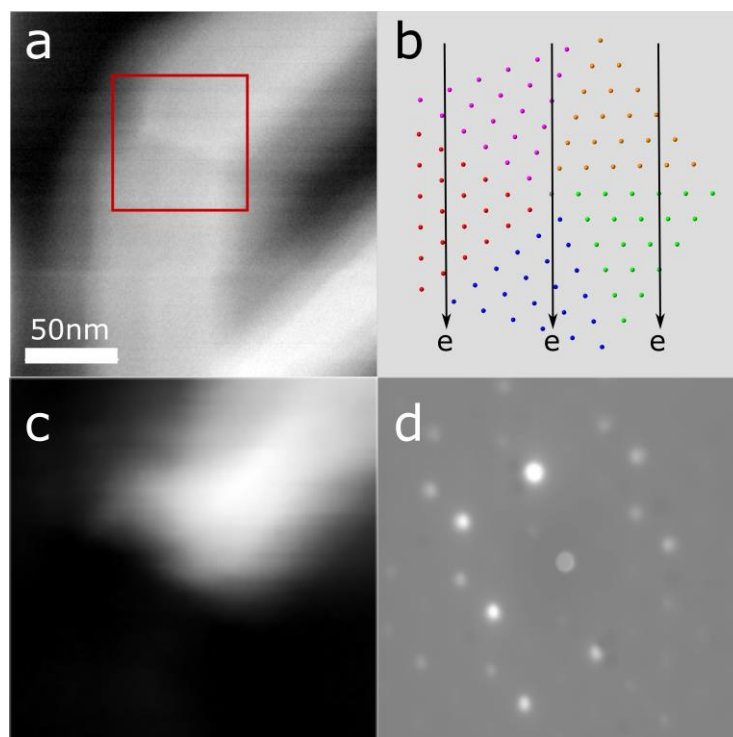


Figure 1. Structure analysis of penta-twinned silver nanowire a) virtual image of the wire (highlighted region used for decomposition). b) Overall wire orientation with respect to the electron beam direction. c) and d) decomposed factor and loading respectively for one [114]-oriented twin segment in the upper part of the wire.