3D Bragg CDI of five-fold twinned Au nanoparticles

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Pentagonal bipyramid gold crystals have attracted the interest of scientists for many decades due to their apparent five-fold symmetry [1]. Closer inspection reveals that the nanocrystals must be composed of five distinct tetrahedral units separated by twin planes in order to exist [2]. Joining such five tetrahedral domains along their [110] axis leaves however a gap of 7.35° so that a solid could in principle not be formed. The mechanism of the stabilisation of these nanocrystals has been subject of debate and is expected to involve a complex stress state [3].

Here we use a combination of Laue micro-diffraction and 3D Bragg Coherent Diffraction Imaging (CDI) to shed light on the crystallography of pentagonal bipyramid Au crystals of 600nm in size (Fig. 1a). We show how the predicted five tetrahedral domains can be individually indexed in the Laue data and display features characteristic of a Σ3 twinned structure. We further discuss the complex peak shape visible in both the Laue and CDI data (Fig. 1b) and how this relates to the strain stabilising the nanoscrystal shape. Finally, we discuss the ongoing efforts to phase the CDI data, which will eventually allow us to retrieve the full 3D strain tensor of the nanoscrystal revealing the unknowns of its complex nature.

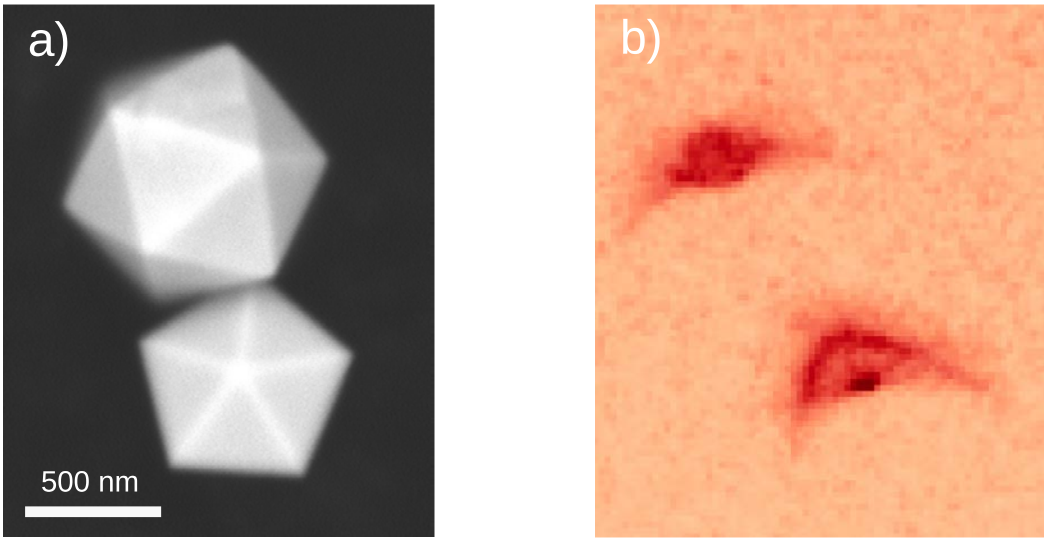

Figure 1: in a) a pentagonal bipyramid crystal is visible on the bottom left corner of the SEM image. The crystals are deposited on an Si substrate. In b), the complex shape of the Laue microdiffraction peaks is visible.

References

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