Study of structural distortions in Eshelby twisted InP nanowires by precession electron diffraction

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Although the huge recent progress of transmission electron microscopy, it is still quite challenging to analyze precisely defects and related lattice deformations inside individual nano-objects. The small size of nanosystems and the complex dynamical diffraction effects renders rather difficult the understanding of real- or reciprocal space studies. Associating the nanometer wide probes and the quase-kinematical diffraction intensities generated by Precession Electron Diffraction (PED), we obtain a remarkable tool to study crystals with high spatial resolution. .

Here, we describe a thorough analysis of structural distortions present in InP NWs (30-40 nm in diameter, wurtzite structure) grown using the Vapor-Liquid-Solid (VLS) mechanism inside a Chemical Beam Epitaxy (CBE) reactor. The wires growth direction is along the [0001] axis and, they contain a screw dislocation aligned with the wire axis. Also, to attain mechanical stability, the crystal develops a backwards torsion in order to compensate the dislocation torque (Eshelby twist predicted in the fifties). The crystal is distorted in a complex, but interestingly systematic way: the basal planes form a helicoid due to the screw dislocation and, also, basal cell vectors are continuously rotating around the *c*-axis along the wire (see Fig 1a). Experiments were realized in Philip CM300 field emission gun (FEG) microscope operated at 200 kV; measurements and analysis were run using a NanoMEGAS ASTAR.

The wires are very thin wires and long (10-20 microns); they are often bent on TEM grid. We have estimated crystal rotation with high precision combining real and reciprocal space information. The 3D curvature wire shape was built by following the hexagonal *c*-axis pixel by pixel along the wire and, also, we isolated the basal plane rotation component from the PED orientation map (Fig. 1b). The derived twist rate is higher (~1.4x) than expected from classical elastic theory probably due to modifications of mechanical behavior in the nanosize regime (ex. surface effects). Within the classical model, the crystal torsion is directly proportional to Burgers vector, which indicates the need to quantitatively estimate this vector from an independent measurement. By analyzing subtle deviation of the hexagonal c-axis in relation to the wire axis (helicoid pattern), we have been able to characterize the screw dislocation with great detail (direction, sense and handedness). Finally, associating a careful assessment of the dislocation induced distortion with full dynamical electron calculations; we observe that our results are compatible with a Burgers vector modulus equal to one hexagonal lattice cell parameter. This study represents a good illustration of the high relevance of spatially resolved PED to characterize subtle structural distortions in individual nanostructures.

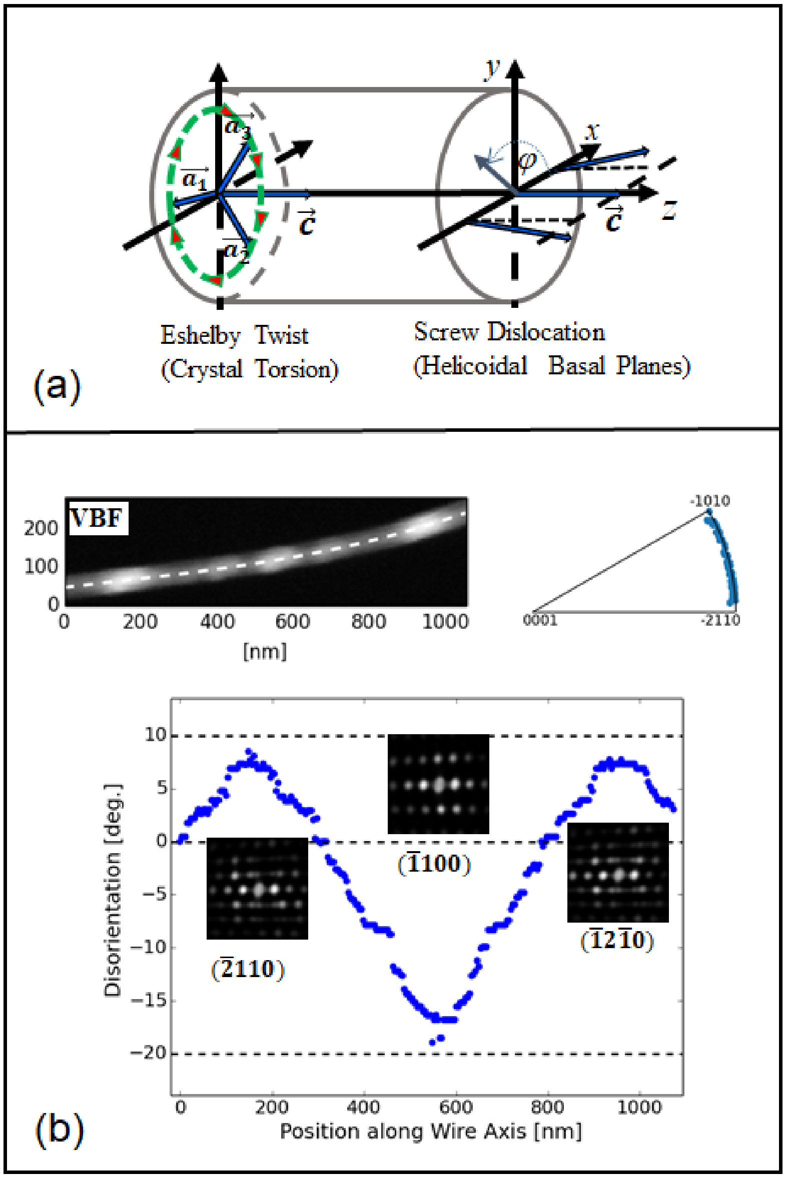

Figure 1. a) Schematic draw showing the structural distortion present in an Eshelby twisted nanowire: continuous rotation of the basal plane base vectors (left) and a disorientation of the c-axis in relation to wire geometrical axis (screw dislocation, right). b) Change of orientation associated exclusively to the rotation of the basal plane component *(hki0)* versus the position along wire; Virtual bright field image, and inverse pole figure orientation are also shown.