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Core Structure of Dissociated Dislocations in Bi_2Te_3 Nanowires

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The weak interlayer bonding and possibilities for large Burgers vectors in Bi_2Te_3 and related layered chalcogenides raise interesting questions regarding the structure of dislocations in these materials. The most extensively studied type of dislocation in Bi_2Te_3 possesses a Burgers vector of type $\frac{1}{3} < 2\overline{1}\overline{1}0 >$. This defect lies in the basal plane and can move easily by glide [1,2]. However, as illustrated in Figure 1, the structure can also incorporate dislocations with a large Burgers vector component lying normal to the basal plane.

In this presentation, we discuss HAADF-STEM observations we have made of such defects in electrochemically deposited nanowires of Bi_2Te_3 [3]. The analysis presented here was made in the course of a broader study exploring how growth and annealing conditions control the resulting crystallinity and internal microstructure in Bi_2Te_3-based nanowires being developed for thermoelectric applications [4,5]. We focus specifically on understanding the core structures of $\frac{1}{3} < 01\overline{1}\overline{1} >$ dislocations, which possess a remarkably large Burgers vector of 1.048 nm. Figure 2 shows an array of such defects forming a low angle tilt boundary near the center of a nanowire. This array efficiently accommodates the misorientation of the Bi_2Te_3 basal planes, which here is about 5.5°, by removing a "half plane" consisting of a Bi_2Te_3 quintuple unit for each dislocation.

Higher magnification imaging (Figure 3) shows that the cores of the $\frac{1}{3} < 01\overline{1}\overline{1} >$ dislocations are dissociated into pairs of partial dislocations that bound an intermediate faulted region. Circuit analysis shows that the partial dislocations are of type $\frac{1}{15}[05\overline{5}\overline{2}]$ and $\frac{3}{15}[000\overline{1}]$. Analysis of the magnitudes of the perfect and partial dislocations suggests that the dissociation is driven in part by the ability of the partial dislocations to reduce the strain energy of the initial $\frac{1}{3}[01\overline{1}\overline{1}]$ dislocation. The vertical alignment of the quintuple layers on either side of the faulted region can vary, as is seen by comparing Figures 3a and 3b. This change in the alignment can arise through glide of the $\frac{1}{15}[05\overline{5}\overline{2}]$ partial dislocation on an inclined $\{01\overline{1}5\}$ type plane. The intermediate faulted region forms a seven plane thick, *septuple* unit, consistent with a local patch of Bi_3Te_4, rather than the normal Bi_2Te_3 quintuple layer structure. As we discuss, these observations suggest a mechanism for accommodating tellurium deficiency, which can arise, for instance, through post-growth thermal treatments.

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[6] Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

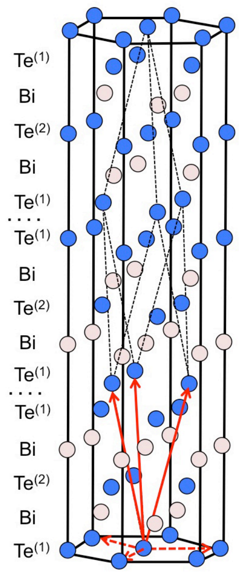

Figure 1. Bi_2Te_3 crystal structure. Burgers vectors of the $\frac{1}{3} < 2\bar{1}\bar{1}0 >$ and $\frac{1}{3} < 01\bar{1}\bar{1} >$ dislocations are indicated, respectively, by the dashed and solid red arrows.

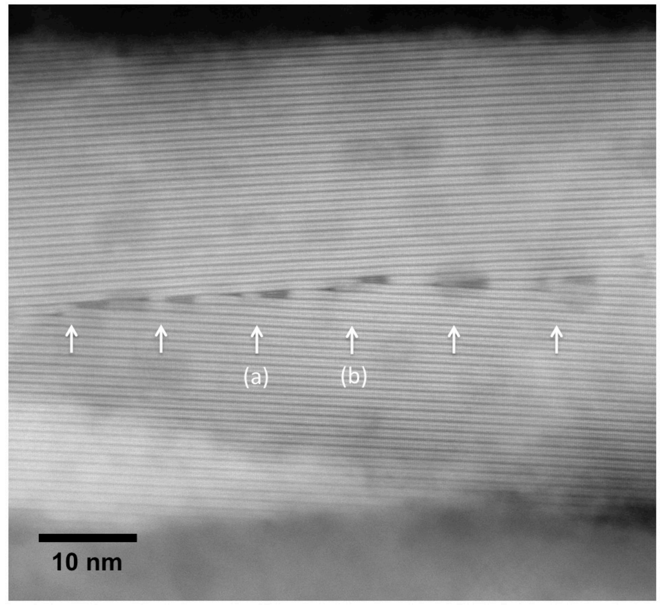

Figure 2. HAADF-STEM image of a Bi_2Te_3 nanowire. A low angle grain boundary, vicinal to the (0001) planes, runs horizontally across the middle of the wire. Tilt misorientation between the grains is accommodated by an array of dissociated $\frac{1}{3} < 01\bar{1}\bar{1} >$ dislocations, which are indicated by arrows.

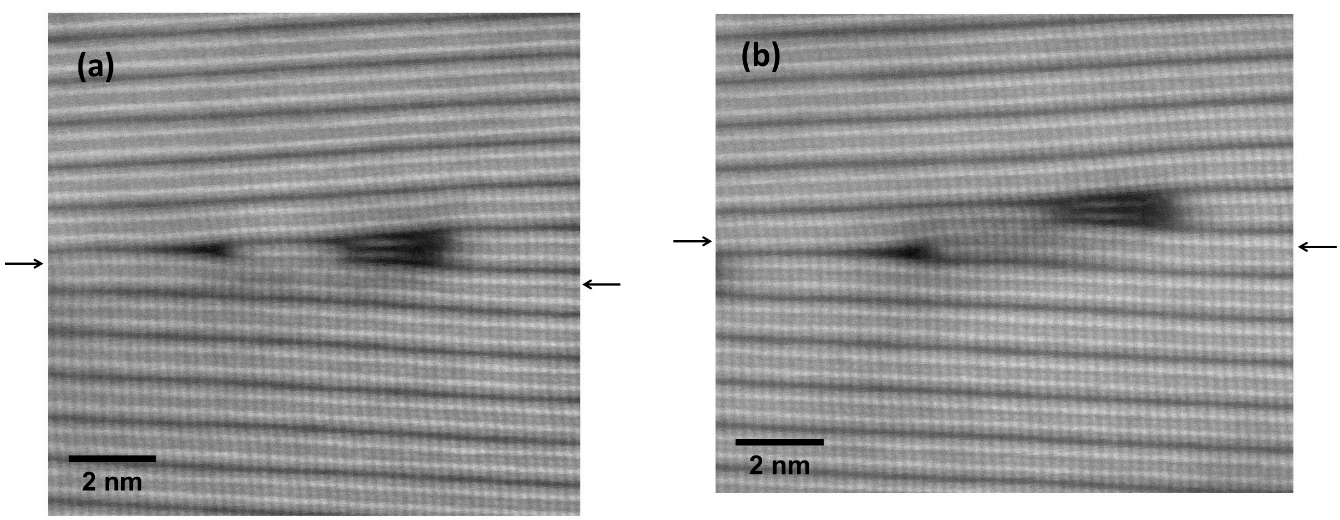

Figure 3. Higher magnification view of the dislocation cores marked as (a) and (b) in Figure 2. The specimen is imaged along a $< 10\bar{1}0 >$ type orientation. In both cases partial dislocations, of type $\frac{1}{15}[05\bar{5}\bar{2}]$ and $\frac{3}{15}[000\bar{1}]$, bound a 7-layer Bi_3Te_4 fault. The two cores differ in the offset of the Bi_2Te_3 quintuple units on either side of the fault. In (a) the lower quintuple unit remains continuous through the fault region; in (b) the quintuple units are offset by two planes.