doi:10.1017/S1431927614007168
Microsc. Microanal. 20 (Suppl 3), 2014

An Electron Microscopic Investigation of (1/3) $<0\bar{1}11>$ Dislocations in Bi_2Te_3 Nanowires: Defect Crystallography and Relationship to 7-layer Bi_3Te_4 Defects.

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Bi_2Te_3, and its iso-structural siblings such as Bi_2Se_3 and Sb_2Te_3, have long been of interest for thermoelectric applications and in recent years have gained prominence in the burgeoning field of topological insulators. It is important to understand the nature of dislocations in these materials since such extended defects are closely connected to the materials growth processes and can affect the thermal and electronic transport properties. The layered structure and possibility for large Burgers vectors in these compounds also raises interesting questions regarding the manner in which dislocations might dissociate.

In this presentation, we discuss electron microscopic observations of $\frac{1}{3}<0\bar{1}11>$ dislocations in nanowires of Bi_2Te_3. There is significant interest in the growth of Bi_2Te_3-based nanowires, motivated by long-standing theoretical predictions of enhanced thermoelectric properties arising in low-dimensional structures of Bi_2Te_3 [1]. 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 [2,3].

Figure 1 shows a low magnification HAADF-STEM image several Bi_2Te_3 nanowires. An enlargement of a dislocation observed in the region indicated by the white box is shown in the higher resolution image shown in Figure 2. Circuit analysis shows that this defect possesses a Burgers vector of *b*= $\frac{1}{3}[01\bar{1}\bar{1}]$. The magnitude of this Burgers vector is remarkably large (1.048 nm) and, as we discuss, drives the dissociation of the defect partial dislocations in order to reduce the strain energy. The dissociated region is 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. The existence of these small patches is consistent with the material accommodating small losses of Te during the annealing process by forming locally Bi-rich defects. Figure 3 shows schematically the stacking arrangements at the defects. As we discuss, the formation of the intermediate Bi_3Te_4 configuration can be understood by analyzing the crystallographic parameters of the bounding partial dislocations. These observations also point to the role that $\frac{1}{3}<0\bar{1}11>$-type dislocations can play in accommodating misorientation at low angle grain boundaries in Bi_2Te_3 and related tetradymite-type compounds [4].

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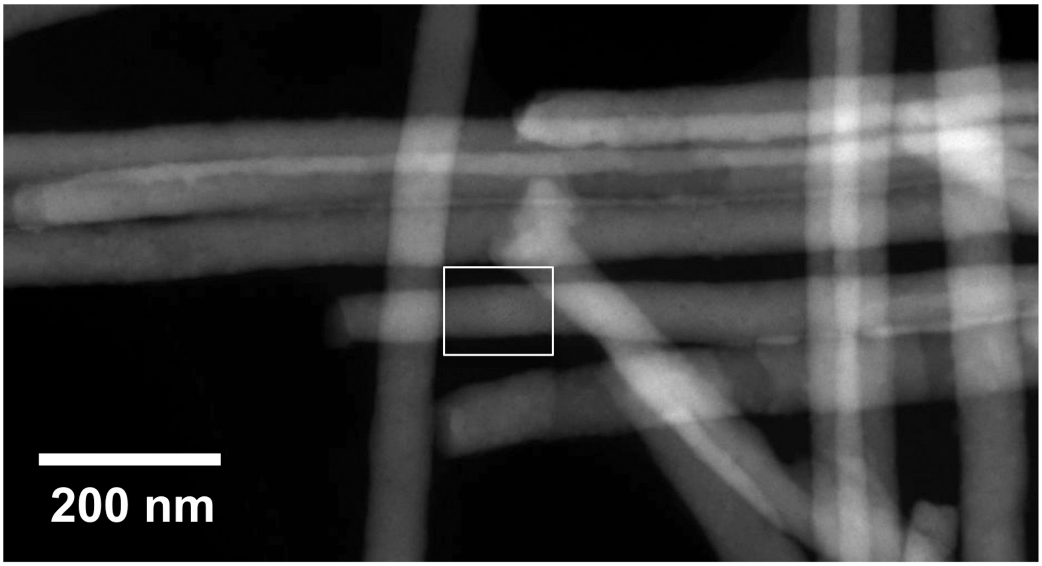

Figure 1. HAADF-STEM image showing several overlapping Bi_2Te_3 nanowires. The white box indicates the area of the dislocation shown in Figure 2.

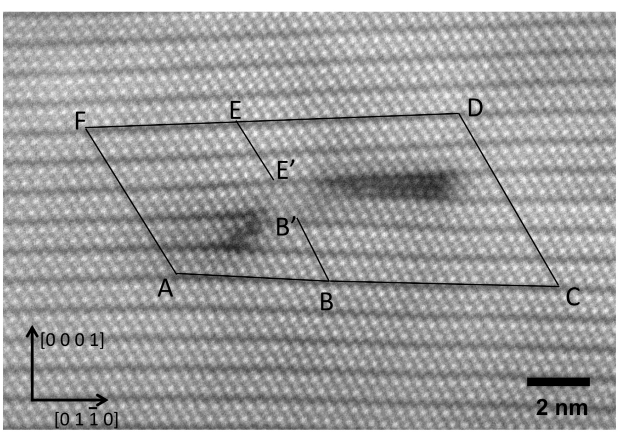

Figure 2. HAADF-STEM showing enlargement of dissociated dislocation ($\boldsymbol{b}= \frac{1}{3}[01\bar{1}\bar{1}]$). Circuit analysis finds that the left and right partial dislocation have Burgers vectors of $\boldsymbol{b}_{\text{left}}=\frac{1}{15}[055\bar{2}]$ and $\boldsymbol{b}_{\text{right}}=\frac{3}{15}[000\bar{1}]$.

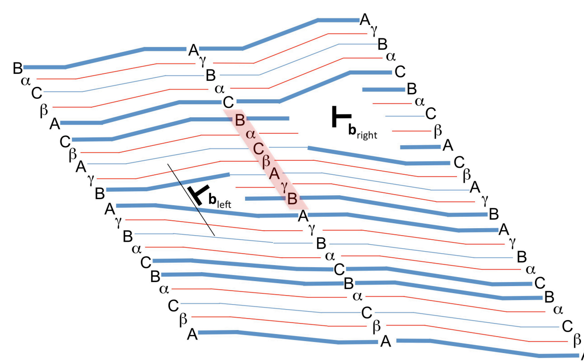

Figure 3. Schematic of stacking arrangements at the dissociated dislocation. The core region consists of a 7-plane layer consistent with Bi_3Te_4. Bi planes are in pink and indicated by Greek letters. Te planes are in blue and indicated by Roman letters.

https://doi.org/10.1017/S1431927614007168 Published online by Cambridge University Press