

Intrinsic Helical Twist and Chirality in Ultrathin Tellurium Nanowires

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Monoelemental nanomaterials with lattice anisotropy are emerging candidates for nano-electronics devices. Exciting properties emerge with non-centrosymmetric crystallinity such as anisotropic thermal conductivity, spin texture, and gyrotropic effects. Nanostructured trigonal tellurium (t-Te) is an air-stable promising candidate for new nanotechnologies due to its high hole mobility, high current density, and predicted larger electronic bandgap compared to the bulk, making it a useful channel material for extremely scaled FETs.¹ The inherent one-dimensional (1D) crystalline structure of Te consists of covalently bonded atoms in a helical chain arrangement along the z-axis with right- or left-handed (P3121 or P3221 space group respectively) chirality. Handedness also provides possible optics and plasmonic applications, making ultrathin (sub 10 nm) Te a versatile material. The preferentially driven growth of Te along the helical chain axis promotes the formation of 1D nanostructures such as nanoribbons, nanotubes, and nanowires (NWs). Nanoscaled chirality provides a means to tune specific responses as the properties become orientation-dependent; however, atomic chirality is rarely expressed at the nanoscale. Several methodologies have been implemented in various types of NWs to express chirality beyond the unit cell by the spontaneous/controlled formation of screw dislocations,² or by directing the handedness with chiral biomolecules³ to promote a periodic helical twist along the axis of the NW. In this presentation, helicity and chirality of ultrathin Te NWs were identified using four-dimensional scanning transmission electron microscopy (4D-STEM) and second harmonic generation circular dichroism (SHG-CD). The subtle changes in orientation along the axis of the nanowire show a previously undetected helical twist along the length axis with enough periodicity to produce nanoscaled ordered chirality. Lattice rotation along the NW's axis was identified with a custom-made postprocessing automated crystal orientation mapping (ACOM) script by template matching the nanobeam electron diffraction (NBED) patterns in the 4D-STEM dataset with a library of possible orientations.⁴ Additional analysis using a classification method of common NBED patterns into classes provides complementary information by increasing the signal-to-noise ratio and compensate for artifacts related to weak scattering of the ultrathin NWs. Orientation changes were more reliably detected in the averaged classes over individual NBED patterns. Evidence of reciprocal lattice rotation from the [2-1-10] to the [10-10] zone axis about the [0001] direction was observed with an approximate twist rate of 0.2-0.3° nm⁻¹. Circular-polarization dependent SHG response confirms the net chirality of randomly-ordered bundles of twisted ultrathin Te NWs; by contrast, as-grown 2D Te nanosheets do not exhibit any net SHG-CD above the uncertainty level.⁵

References

1. Kramer, A.; Van de Put, M. L.; Hinkle, C. L.; Vandenberghe, W. G., Tellurium as a successor of silicon for extremely scaled nanowires: A first-principles study. *npj 2D Materials and Applications* **2020**, *4* (1), 10-1-8.

2. Sung, B.; de la Cotte, A.; Grelet, E., Chirality-controlled crystallization via screw dislocations. *Nature Communications* **2018**, 9 (1), 1405-1–7.
3. Ben-Moshe, A.; Wolf, S. G.; Sadan, M. B.; Houben, L.; Fan, Z.; Govorov, A. O.; Markovich, G., Enantioselective control of lattice and shape chirality in inorganic nanostructures using chiral biomolecules. *Nat. Commun.* **2014**, 5 (1), 4302-1–9.
4. Hong, X.; Zeltmann, S.; Savitzky, B.; DaCosta, L. R.; Mueller, A.; Minor, A. M.; Bustillo, K.; Ophus, C., Multibeam Electron Diffraction. *arXiv* **2020**, arXiv:2009.09134.
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