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Meeting-report

Exploring the Structure of the Chiral, One-Dimensional Semiconductor InSeI Via High-Resolution Electron Microscopy

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InSeI is a one-dimensional semiconductor that consists of an InSe backbone with iodide ions attached in a spiral. Each individual InSeI "chain" has a handedness due to the chirality of the iodine spiral. While synthesis of this material was first reported in 1980 by Swaitzki et al. [1], very few studies were performed on InSeI in the years following, with most being computation-based. Very recently, experimental studies on InSeI were completed by Choi et al. [2] and Cordova et al. [3]. However, atomic-resolution structure images in this system have yet to be realized, as this was not the purpose of any of the previously mentioned studies. In this work, we studied the structure of InSeI nanoribbons through high-resolution electron microscopy, specifically aberration-corrected transmission electron microscopy (AC-TEM). These measurements were collected in an FEI Titan 80/30 ETEM operated at 300kV using a BM OneView camera.

Figure 1(a) shows models of the atomic structure of InSeI. The top model shows the atomic positions for all three elements present (In (pink), Se (light green), I (purple)), while the bottom panel shows only the iodine atomic positions. The positions of these iodine atoms are what give chirality to each InSeI chain. Figures 1(b) and 1(c) show AC-TEM images of an InSeI nanoribbon oriented along the [1 0 0] zone axis. These images were acquired at 13kX and 380kX, respectively. In Figure 1(c), four distinct regions are identified as follows:

I = vacuum, II = amorphous carbon, III = thin InSeI, IV = thick InSeI.

Bandpass filtering was performed on the FFT of the AC-TEM image in Figure 1(c) to improve the image quality and signal-to-noise ratio. Figure 2(a) shows the result of this process after zooming in to the area of interest (region III in Figure 1(c)). Individual chains of InSeI are observed, with the chain direction running along the c-axis of the nanoribbon. Bright spots located between the InSeI chains are believed to be clusters of iodine atoms that are too closely spaced together to be individually resolved. Some additional details are observed when focusing on individual InSeI chains, but the resolution of the image is not good enough to conclusively identify atomic positions within the chain. Figure 2(b) shows the FFT of Figure 1(c) that was used to generate Figure 2(a). The inner and outer bounds of the bandpass filter ($0.274 nm^{-1}$ and $8.987 nm^{-1}$, respectively) were chosen to include all FFT spots except for the central spot while excluding information beyond the outermost ring of spots. Additional contrast is present in the FFT, which is believed to come from the amorphous carbon support under the InSeI nanoribbon.

To better understand the AC-TEM results, image simulation was carried out using the abTEM package in Python. Simulations were performed using $C_S = -13 \mu m$, $C_C = 1 mm$, and $\Delta f = -40 nm$. A Gaussian blur of 0.8 was also applied to the resulting images to help represent the effects of limited resolution, which would be caused by other effects such as residual aberrations and thermal vibrations. Figure 2(c) shows the result of these simulations. The same quasi-1D structure observed in Figure 2(c) is present, which validates the result of the experiment. Furthermore, the simulated image shows additional detail that suggests the chirality of individual InSeI chains may be able to be determined if higher resolution is achieved.

Further studies using aberration-corrected high-angle annular dark field scanning transmission electron microscopy (HAADF-STEM) are planned to meet this requirement. A combination of electron tomography and ptychographic reconstruction may also be useful for experimentally determining the three-dimensional structure of InSeI [4].

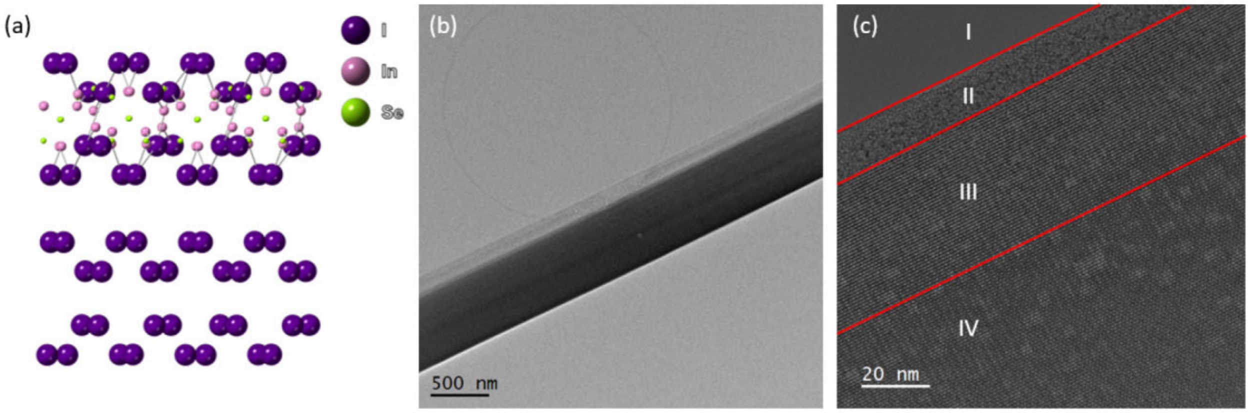

Fig. 1: (a) structural model of InSeI showing all atomic positions (top) and only the iodine atomic positions (bottom). (b) Low-magnification bright-field TEM image of an InSeI nanoribbon oriented along the [1 0 0] direction. (c) 300kX magnification BFTEM image of the same nanoribbon after aberration correction. Different regions of the sample are divided by red lines.

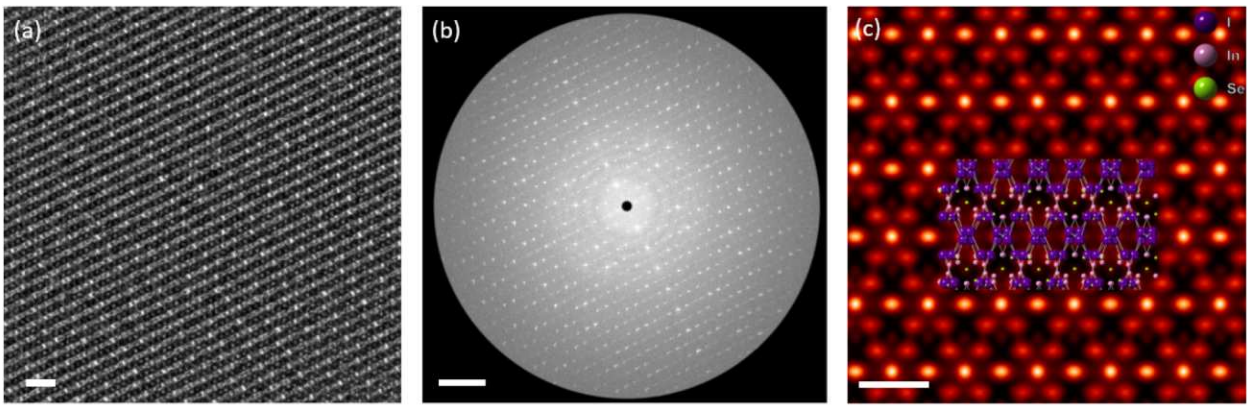

Fig. 2: (a) Zoomed-in version of Figure 1(b) after FFT filtering using a bandpass filter (scale bar = 2nm). (b) Masked FFT of 1(b) that was used to generate Figure 2(a) (scale bar = $2nm^{-1}$). (c) Simulated BFTEM image of a 25nm thick InSeI unit cell, tiled to represent an approximately 5x5 nm^2 area (scale bar = 1nm).

References

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