

Electron diffraction of organic nanowires

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Nano-structured organic materials have recently attracted much attention. Their applications include light-emitting diodes, field-effect transistors, chemical sensors, optical waveguides and lasers, as reviewed recently by Zhao *et al.* [1]. To solve structure of organic nano-materials is not an easy task due to the lack of large size single crystal which can be studied by X-ray diffraction. High sensitivity of the organic structure to radiation damage imposed another difficulty: organic specimens are quickly damaged before a high resolution electron image can be recorded. Organic materials, which consist mostly of light elements like C, O and N, also have low contrast in scanning transmission electron microscopy (STEM) imaging, such as high angle annular dark-field mode which shows Z-contrast. The structure of a thin film phase of pentacene was solved by electron diffraction [2]. In the work, the structure of 1,5-diaminoanthraquinone (DAAQ) nanowire is studied by electron diffraction.

The DAAQ nanowire arrays were prepared with a physical vapor transport method [3]. Figure 1 shows an SEM image of arrays of DAAQ nanowires deposited at 160 °C for 5 min. The length and diameter of the DAAQ nanowires can be readily controlled by altering conditions. To determine the crystal structure and the growth direction, we collected the electron diffraction patterns in several orientations by tilting the single wire as shown in Figure 2. Figure 3 shows the set of diffraction patterns obtained by continuously rotating the nanowire along its wire axis. The set of titled diffraction patterns enables us to reconstruct the reciprocal lattice and to determine the lattice type and parameters. The reciprocal lattice parameters obtained from the reconstruction are $a^*=0.265 \text{ \AA}^{-1}$, $b^*=0.103 \text{ \AA}^{-1}$, $c^*=0.067 \text{ \AA}^{-1}$, $\alpha^*=\gamma^*=90^\circ$, $\beta^*=97.6^\circ$, which gives a monoclinic lattice with $a=3.78 \text{ \AA}$, $b=9.73 \text{ \AA}$, $c=15.01 \text{ \AA}$, $\beta=82.4^\circ$. The experimentally measured tilting angles among the patterns as well as calculated ones from the reconstructed unit cell were labeled in fig.3. The agreement between the experimental and calculated angles proves the correctness of the reconstructed unit cell. By comparing the diffraction patterns to the TEM image, it is also revealed that the nanowire axis is along the [100] direction (as shown by the arrowhead in Figure 2). There are tangible prospects for solving the atomic structure if large number of kinematic electron diffraction data can be collected, which is underway. The presentation will cover the general strategy for solving crystal structure and crystallography problems in organic and “soft” nanostructures.

References

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- [2] J.S. Wu and J.C. Spence, *J. Appl. Crystallogr.* 37 (2004) 78.
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- [4] This work was performed in the EPIC facility of NUANCE Center at Northwestern University. Research was supported by the Nanoscale Science and Engineering Center at Northwestern (NSF EEC-0647560) and the American Chemical Society Petroleum Research Fund (48678-G10).

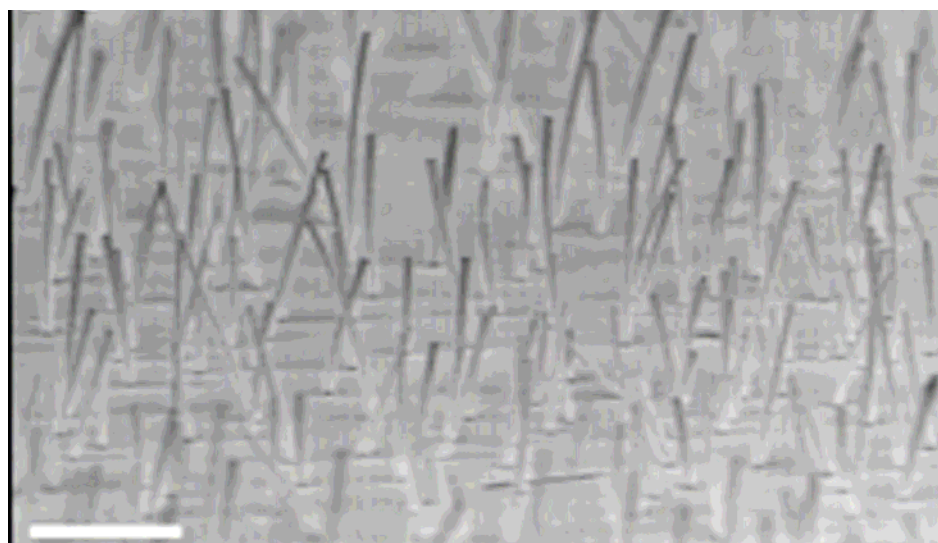


Figure 1. A SEM image of the 1,5-diaminoanthraquinone (DAAQ) nanowire arrays deposited at 160 °C for 5 min. The white scale bars is 1 μ m.

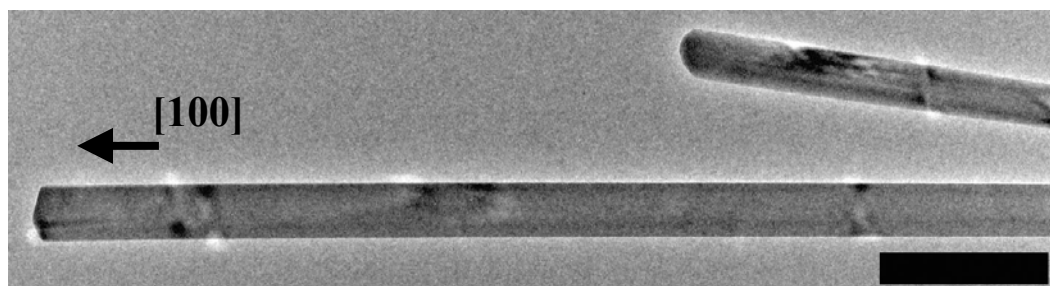


Figure 2. TEM image of the DAAQ nanowire used to obtain the tilted electron diffraction patterns shown in fig.3. The growth direction is identified as along the [100]. The scale bar is 500 nm.

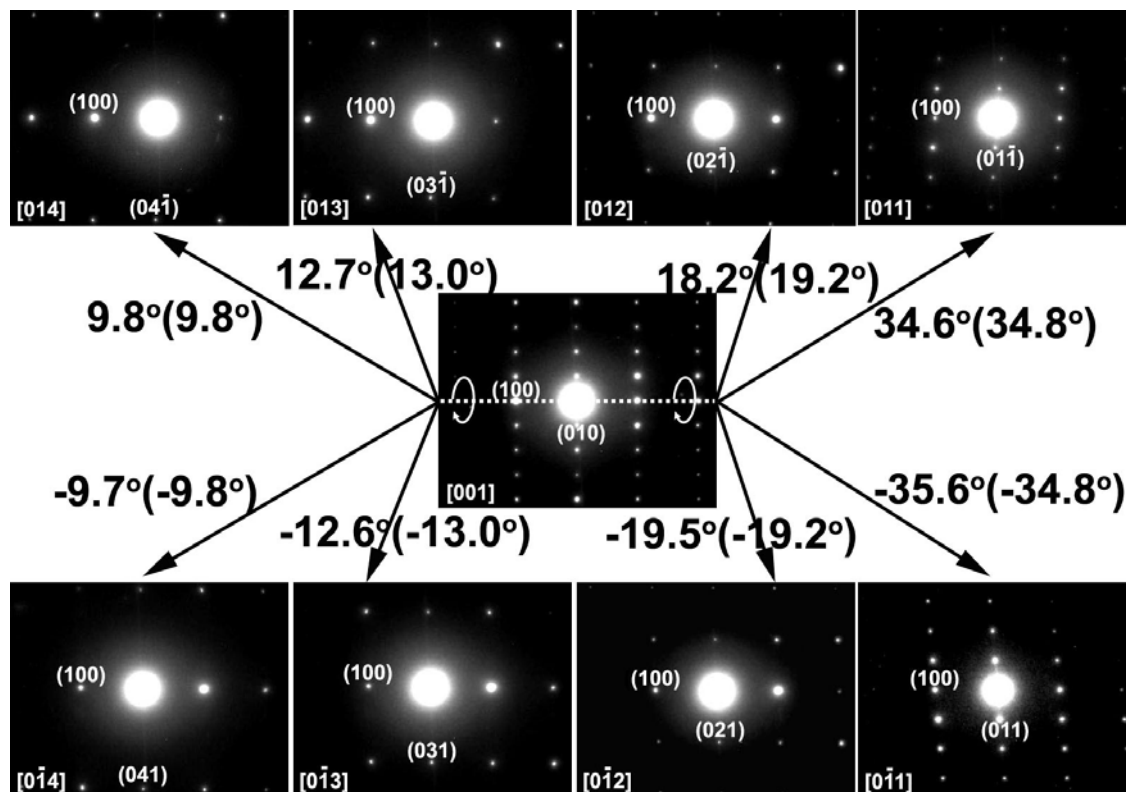


Figure 3. A set of electron diffraction patterns of the same nanowire acquired while tilting the nanowire along its [100] axis. The experimental tilting angles were marked, which can be compared to the angles in parentheses that are theoretical values calculated from the reconstructed unit cell.