

Local Structural Characterization of Gold Nanowires

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Nanowires with aspect ratios 40~70 were synthesized by our previous report. However, synthesis of nanowires alone was not possible, and the fact that particles form in mixed shapes suggests that those gold seeds that can grow preferentially along their longitudinal axes possess a unique crystal configuration to favor an axial growth. Figure 1a shows a typical gold nanowires image. Electron diffraction (inset in Figure 1a) from the single rod shows it to be along the [110] crystallographic zone axis. Electron diffraction analysis of mature nanowires showed superpositions of two specific pairs of crystallographic zones, either $\langle 112 \rangle$ and $\langle 100 \rangle$ or $\langle 110 \rangle$ and $\langle 111 \rangle$, which were consistent with a cyclic penta-twinned crystal with five $\{111\}$ twin boundaries arranged. The nanowires have an idealized 3-D prismatic morphology with ten $\{111\}$ end faces and five $\{100\}$ or $\{110\}$ side faces, or both. This structure was similar to previous result on gold nanorods prepared by seed-mediated growth method in CTAB. TEM image of a single gold nanowire at high resolution is shown in Figure 1b. The HRTEM image reveals that these nanowires show single crystalline nature, as indicated by atomic lattice fringes. Most interestingly, the image provides the direct evidence of twin defect structures on the (100) crystal face (arrowed in Figure 1b). The atomic structural detail in Figure 1b demonstrates that the defects are twin lamellae with the dimension of the lamellae of about 5 nm. This has important implications in the applications of nanowires in the molecular device technology. In the wet synthesis described here, all nanowires were observed to contain the twin defects.

The change of the internal crystal structure is seen in wide angle x-ray diffraction (XRD) studies. Figure 2 shows representative XRD patterns of as-prepared gold nanowires and gold foil, respectively. The XRD patterns of the foil and nanowires were assigned to the (111), (200), (220), (311), and (222) reflections of the face-centered cubic structure of gold. The lattice constant calculated from this pattern was 4.081(3) Å, a value in agreement with the literature report ($a = 4.079$ Å, Joint Committee on Powder Diffraction Standards file no. 65-2870). Note that the standard XRD patterns of nanowires and foil are nearly identical. It is worthwhile to note that the ratio between the intensities of the (220) and (111) diffraction peaks was higher than the conventional value (0.16 versus 0.19), which implied that our nanowires were abundant in $\{110\}$ facets, and thus their $\{110\}$ planes tended to be preferentially oriented parallel to the substrate. Accompanying with the growth of gold, the $\{110\}$ facets increased due to the growth preferentially along their longitudinal axes. This is in accordance with electron diffraction analysis of

mature nanowires, the wires grow along the [110] directions.

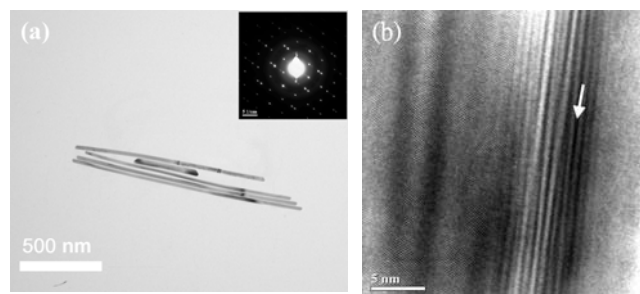


Figure 1. TEM micrographs of gold nanowires. (a) as-prepared nanowires and electron diffraction pattern (inset). (b) HRTEM image of nanowires.

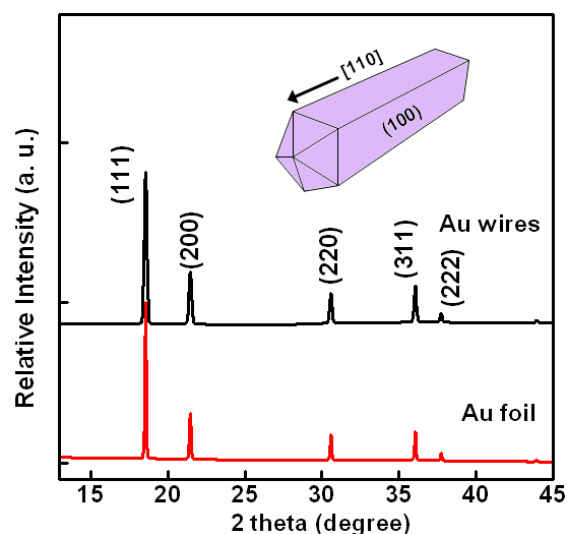


Figure 2. XRD patterns of as-prepared gold nanowires and gold foil.