Electronic Supplementary Information

Defect Segregation and Optical Emission in ZnO Nano- and Microwires

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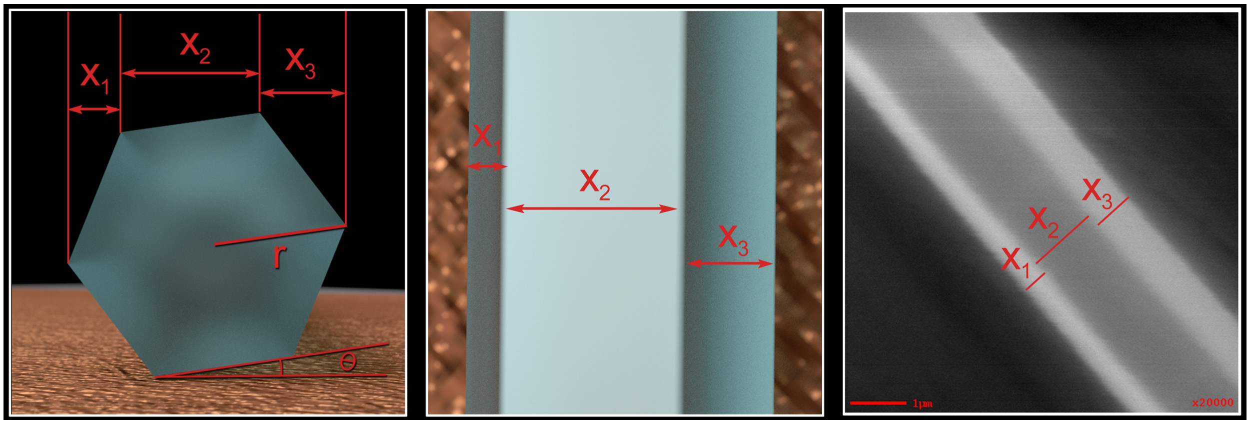

FIG. 1. a) Cross section view of a perfect hexagonal wire showing geometrical parameters (r and θ), and the overhead projected lengths of the facets (x_1, x_2, and x_3) b) The overhead view of a perfect hexagonal wire also showing the same facet lengths. c) Overhead image of hexagonal wire taken with a SEM.

I. EXTRACTING WIRE PARAMETERS

In order to take CL measurements on the ZnO wires measured in this paper we first had to disperse them onto our SEM's sample holder. This results in the wires mostly lying with their c-axis parallel to the sample holder, as depicted in the Fig 1. To analyze the data and run our simulations it was necessary to estimate the geometrical parameters (radius, r, and tilt angle, θ) of the wires, shown in Fig 1(a). For a perfect hexagon, viewed from above, the lengths of the facets are give by,

$$x_1 = \frac{r}{2}(\cos\theta - \sqrt{3}\sin\theta) \tag{1}$$

$$x_2 = r\cos\theta \tag{2}$$

$$x_3 = \frac{r}{2}(\cos\theta + \sqrt{3}\sin\theta) \tag{3}$$

The distances x_1, x_2, and x_3 are also shown in Fig 1. Measuring these distances using a secondary electron image (SEI) allowed us to extract the radius and tilt angle of the wire as well as measure it's regularity. The regularity of the hexagon is quantified by a number we called the deviation, D,

$$D = \frac{\sum_{i=1}^{3} |x_i^{calc} - x_i^{meas}|}{\sum_{i=1}^{3} x_i^{meas}}$$

where, x_i^{meas}, are the measured lengths of the wire's hexagonal facets projected onto the sample plane (using a SEI image), and x_i^{calc} are the theoretical values of these projections calculated using the esimated hexagon radius, r, tilt angle, θ, and equations (1)-(3). A perfect hexagon would have $D = 0$ while, for example, the wire in Fig. 1(c) had $D = 5\%$. Note, Fig. 1(c) is the wire used for the simulation whose results are shown in the main paper's Fig. 4(b). The most regular wires were chosen for the paper's simulation and analysis.