Appendix

Derivation of Equations 3.1, 3.2, and 3.7

The catalyst tip at the top of a VLS-grown wire shown schematically in Figure 3.8a is isolated below in Figure A.1.

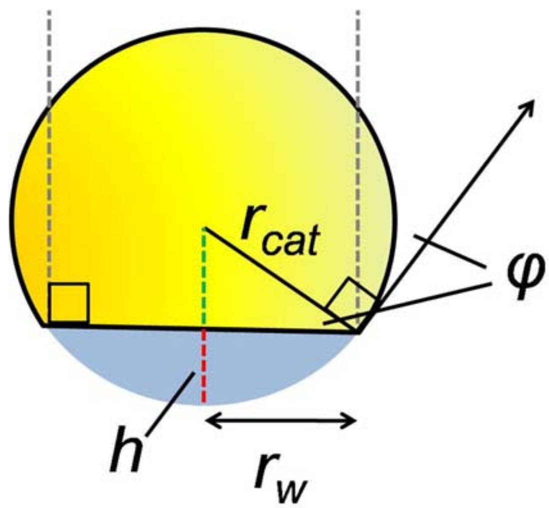

Figure A.1. Schematic of the catalyst tip on a VLS-grown wire.

As Figure A.1 shows, the angle, φ, between the liquid-vapor interface and the direction of wire growth is the same as the angle between r_{cat} (as drawn) and r_w, leading to the relation:

$$r_w = r_{cat} \cos\varphi \qquad \text{(A.1)}$$

which is Equation 3.1 relating the wire radius to the catalyst tip radius. The volume of the catalyst tip, V_{cat}, can be determined by recognizing that the ball is a truncated sphere. The missing section of the sphere, shown in blue in Figure A.1, is a spherical cap. The formula for the volume of a spherical cap is known and is (using the variables in Figure A.1):

$$V_{spherecap} = \frac{\pi}{6}\left(3r_w^2 + h^2\right)h \qquad \text{(A.2)}$$

Where $V_{spherecap}$ is the volume of the spherical cap, h is the height of the cap, and r_w is the radius of the cap (equal to the VLS-grown wire radius in this case). Recognizing that:

$$\sin\varphi = \frac{r_{cat} - h}{r_{cat}} \qquad \text{(A.3)}$$

and rearranging gives:

$$h = r_{cat}\left(1 - \sin\varphi\right) \qquad \text{(A.4)}$$

The catalyst tip volume is the volume of the entire sphere minus the spherical cap:

$$V_{cat} = \frac{4}{3}\pi r_{cat}^3 - \frac{\pi}{6}\left(3r_w^2 + h^2\right)h \qquad \text{(A.5)}$$

Substituting into Equation A.5 with Equations A.1 and A.4 yields:

$$V_{cat} = \frac{4}{3}\pi r_{cat}^3 - \left[\frac{\pi}{6}\left(3r_{cat}^2\cos^2\varphi + r_{cat}^2\left(1-\sin\varphi\right)^2\right)r_{cat}\left(1-\sin\varphi\right)\right] \qquad \text{(A.6)}$$

which simplifies to Equation 3.2:

$$V_{cat} = \frac{4}{3}\pi r_{cat}^3\left[1 - \frac{1}{8}\left(3\cos^2\varphi + \left(1-\sin\varphi\right)^2\right)\left(1-\sin\varphi\right)\right] \qquad \text{(A.7)}$$

The truncated-cone shape of Figure 3.8b that is etched into the oxide buffer layer of the substrate is shown again in Figure A.2. Because the buffered HF etches SiO_2 isotropically, it etches to the side at the same rates it etches downward. This gives the sloping edge a 45° angle and makes the height of the cone equal to its radius. The volume of the truncated cone that will be occupied by catalyst is equal to the entire cone minus the imaginary extended cone tip that would project beyond the oxide layer:

$$V_{cat} = \frac{1}{3}\pi\left(t_{cat} + r_h\right)^3 - \frac{1}{3}\pi r_h^3 \tag{A.8}$$

which simplifies to Equation 3.7:

$$V_{cat} = \frac{1}{3}\pi\left[t_{cat}^3 + 3t_{cat}^2 r_h + 3t_{cat} r_h^2\right] \tag{A.9}$$

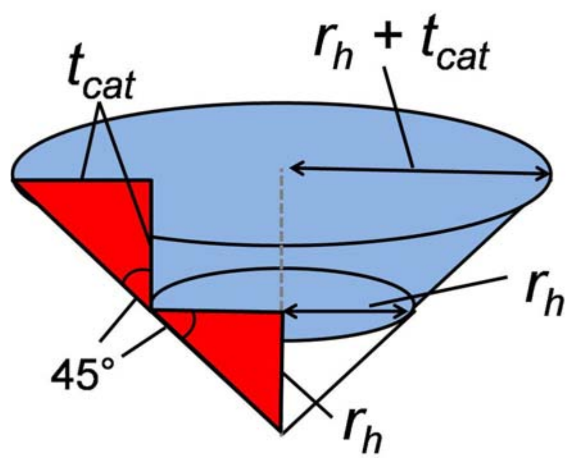

Figure A.2. Schematic of the truncated-cone hole etched into the buffered oxide layer.