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Supplementary Information for “Structural Evolution and Carrier Scattering of Si Nanowires as a Function of Oxidation Time”

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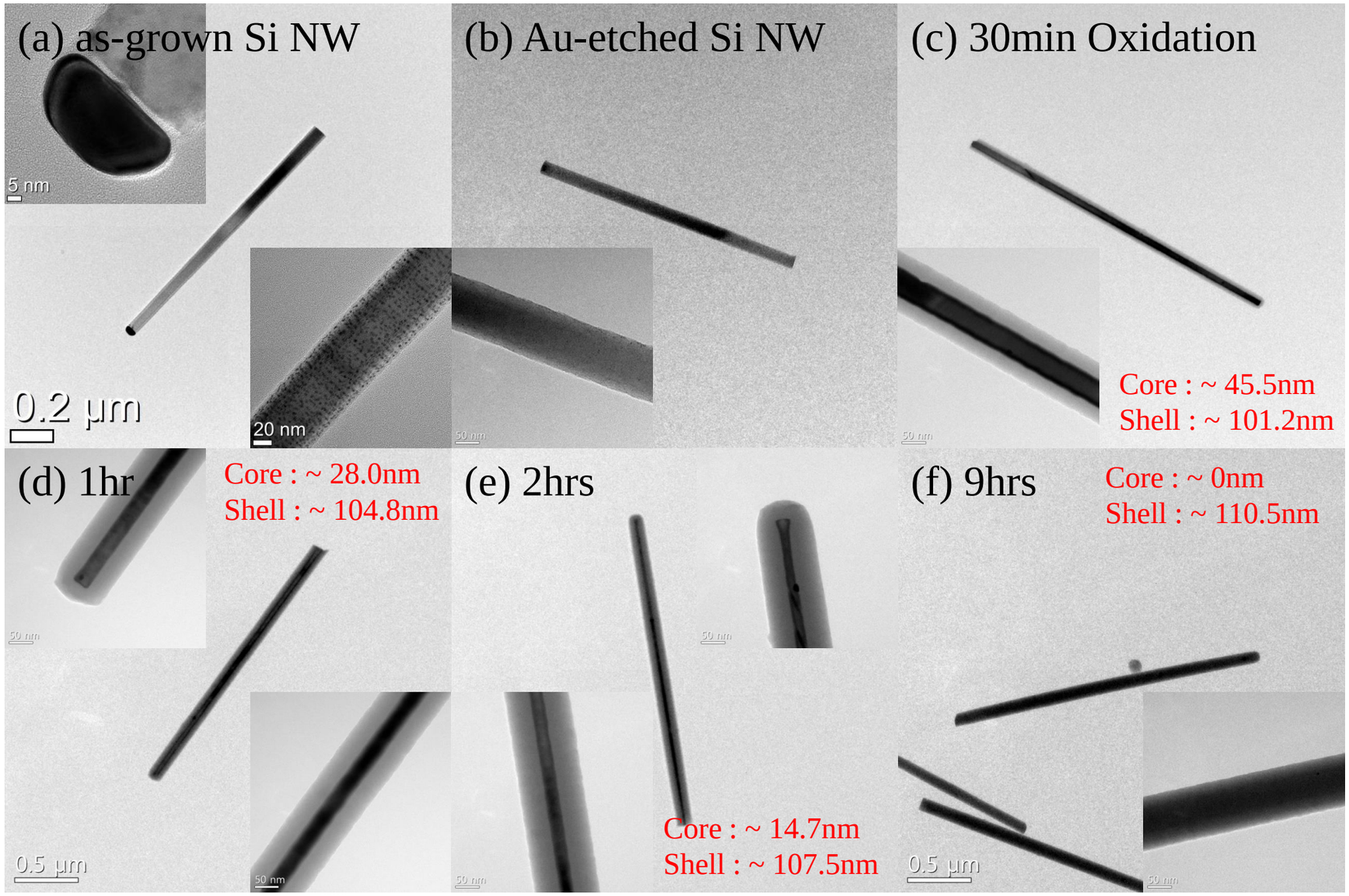

Figure S1. TEM images of Si NW (a) and Au-etched Si NW (b). The oxidation process involved treating Au-etched Si NWs at a temperature of 900 ℃ with the the oxidation time varied from 30 min (c), 1 hr (d), 2 hrs (e), and 9 hrs (f). They formed a Si/SiO_2 core/shell structure: the Si core became thin while the SiO_2 shell thickens as the oxidation time increased.

Supporting Figure S1.

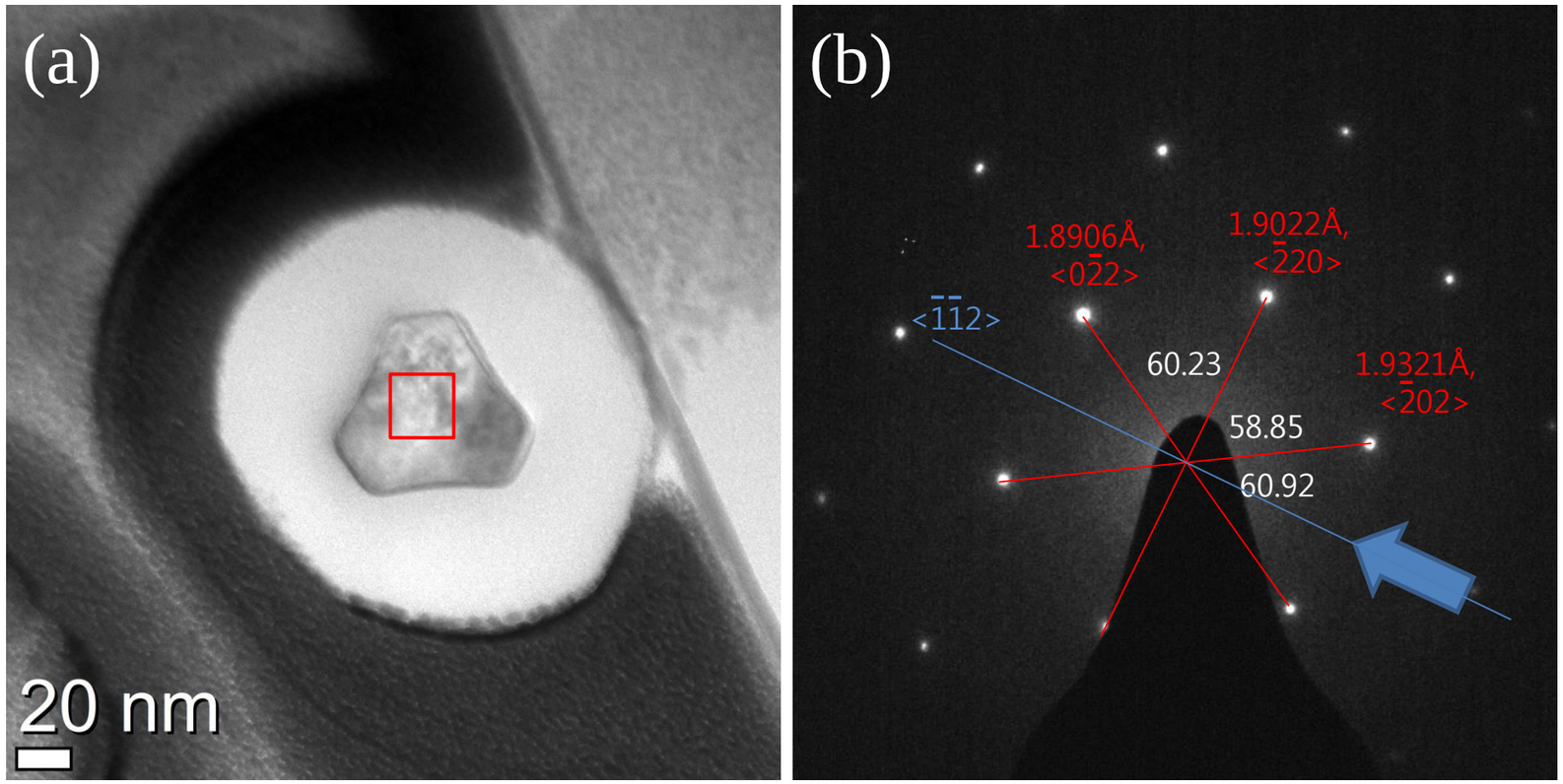

Figure S2. TEM image and selective area electron diffraction pattern of the cross-sectional shape of oxidized Si NW. The Si NW was grown in the [111] direction (a) and six side direction revealed {112} facets.

Supporting Figure S2.

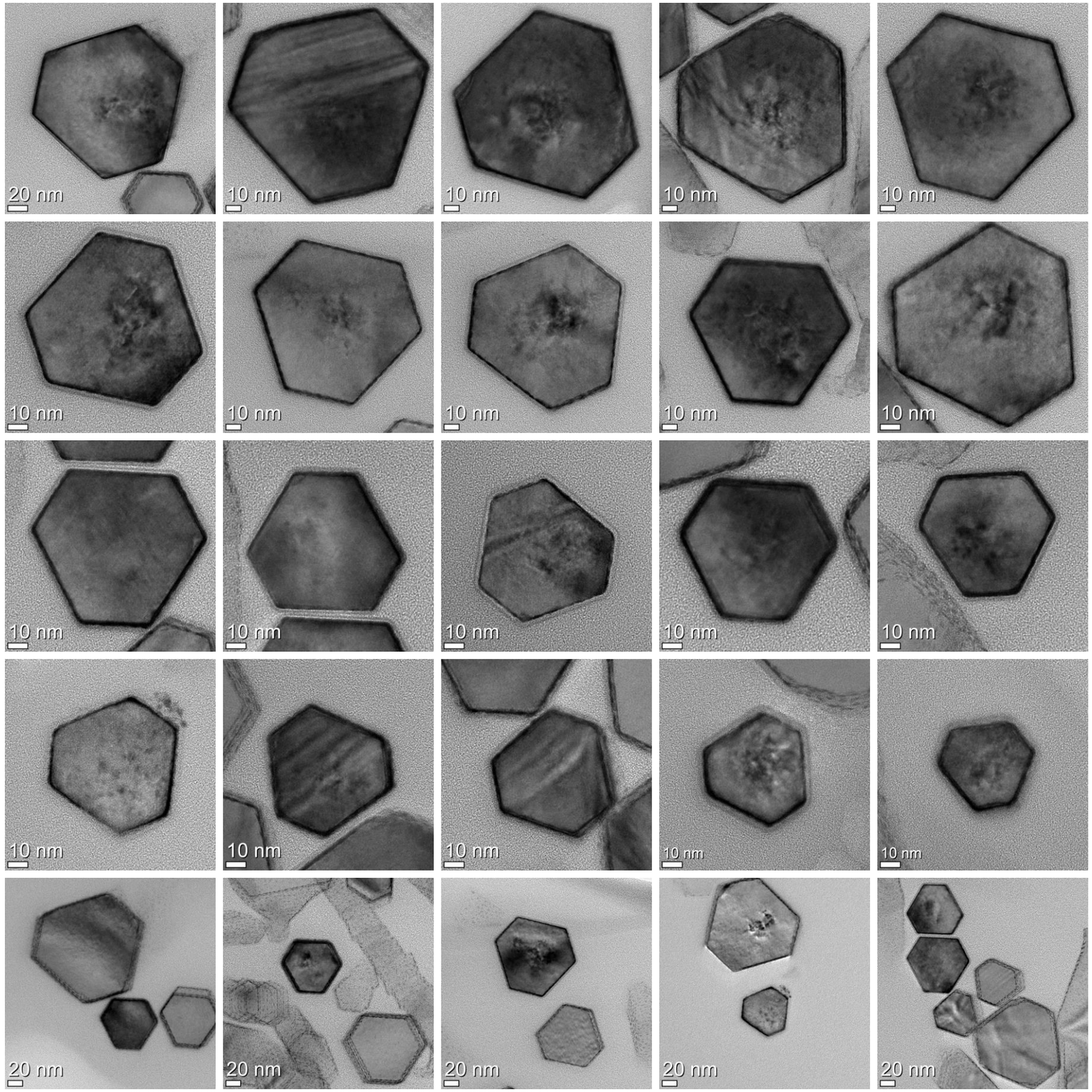

Figure S3. HR-TEM images of the cross-sectional shape of as-grown Si NWs. To investigate whether 3-fold symmetry shape depends on diameter, we observed the cross-sectional shape of numerous Si NWs.

Oxidation time	Average of ‘D’ (nm)	STDEV of ‘D’ (nm)	Number of nanowires
As-grown	82.5	16	100
30 min	86.6	11.51	58
1 hr	85.3	13.3	63
2 hr	84.4	10.6	55
9 hr	82.8	10.4	53

Table S1. Summary of the calculated initial diameters from the oxidized Si NWs as a function of oxidation time.

Supporting Table S1.

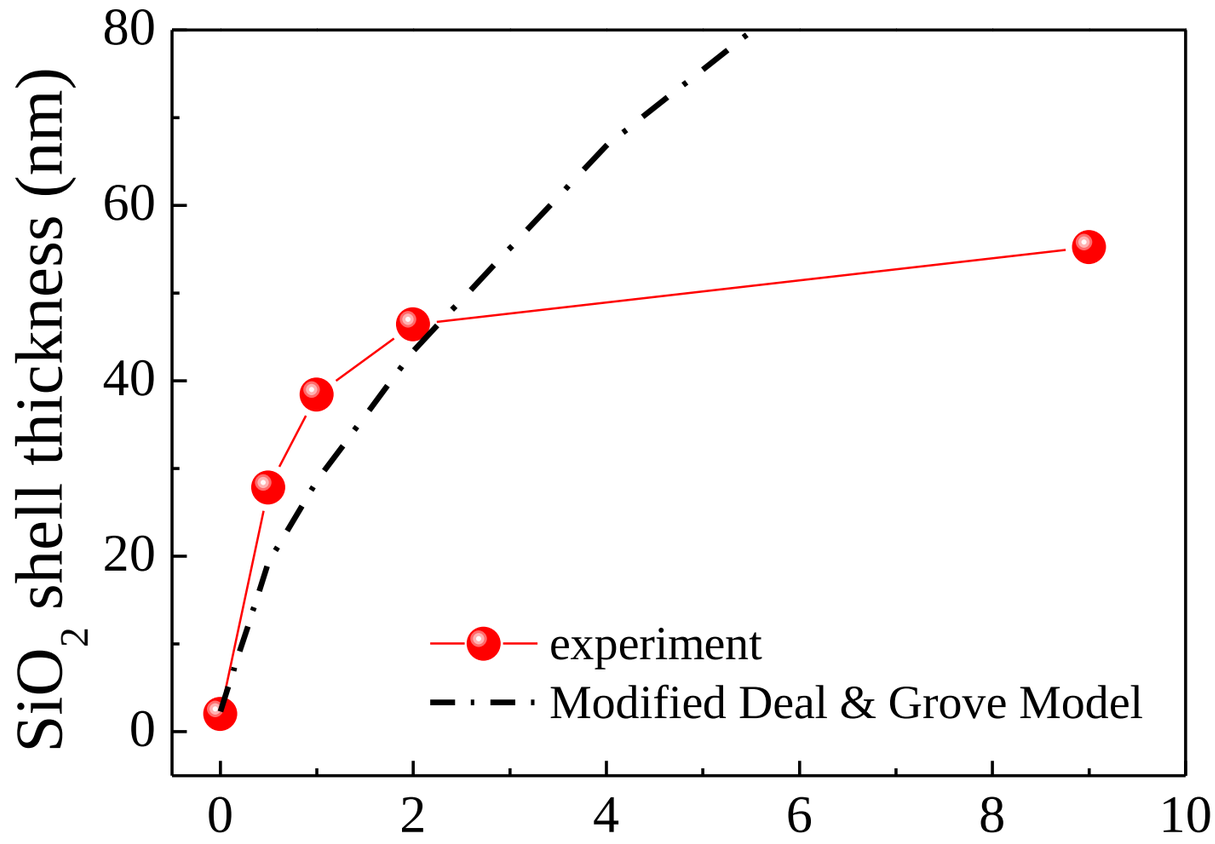

Figure S4. Based on the results in Table S1, the SiO_2 shell thickness formed at Si NWs with similar initial diameters are measured as a function of oxidation time. The tendency of SiO_2 shell thickness to change depending on oxidation time is shown in graphically. Moreover, the change in SiO_2 shell thickness as a function of oxidation time was compared with modified Deal-Grove curve [32].

Supporting Figure S4.

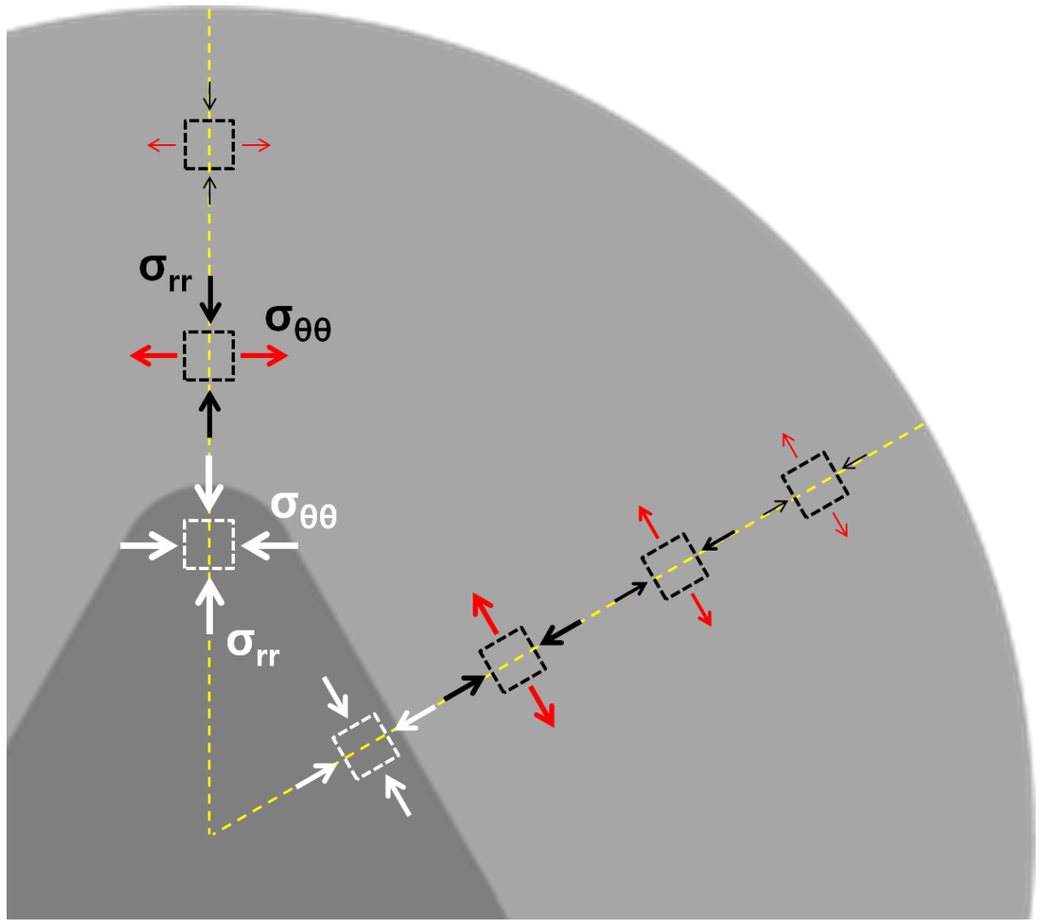

Figure S5. The schematic diagram presenting the stress component. In the case of a SiO_2 shell, compressive stress is induced along the perpendicular direction while tensile stress occurs parallel to the interface of Si/SiO_2, and in case of the Si core, compressive stress is induced along both the perpendicular and parallel directions to the interface of Si/SiO_2.

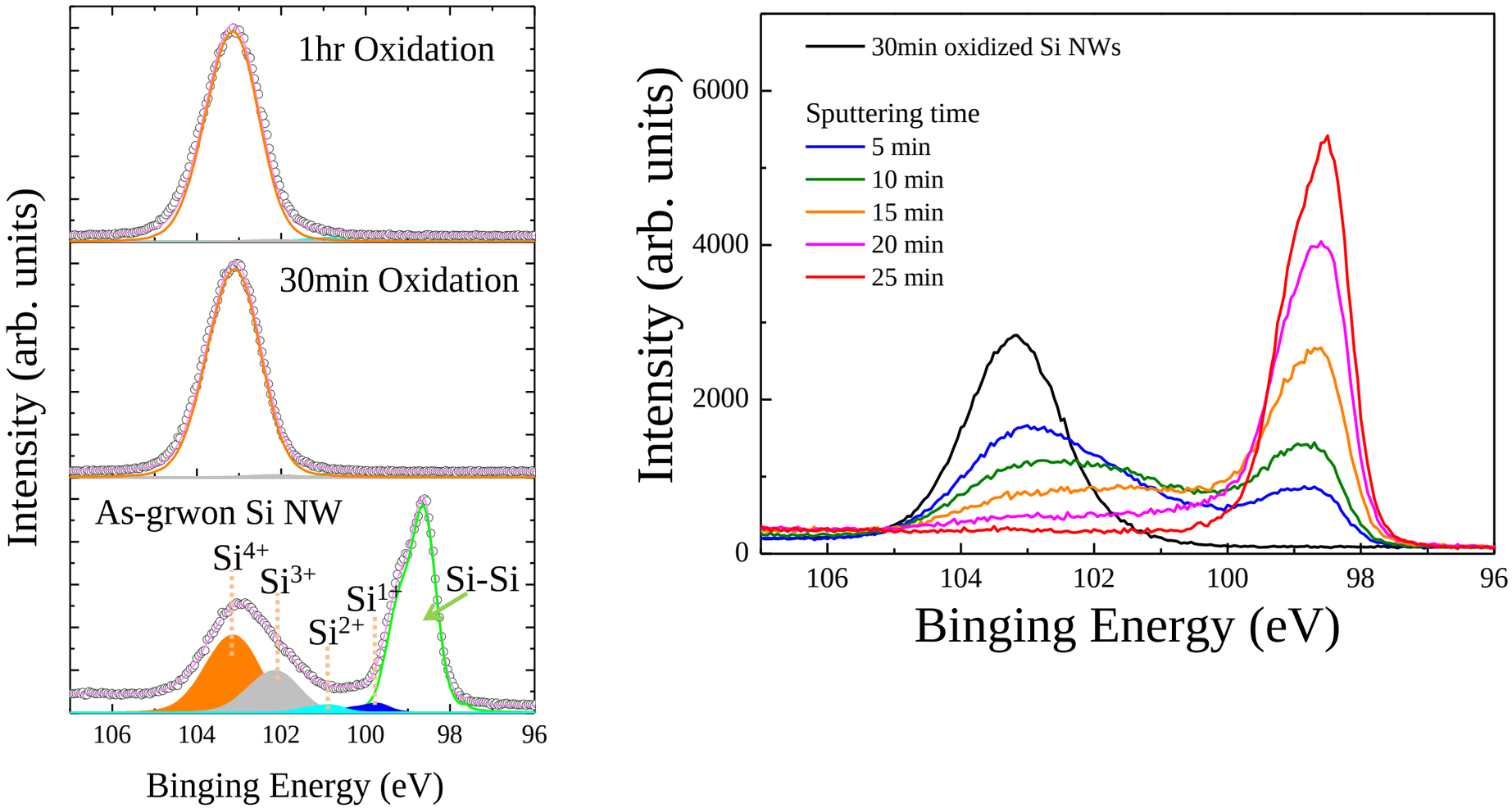

Figure S6. **Left**: The XPS spectra for Si 2*p* core-level obtained from the as-grown and oxidized Si NWs as a function of oxidation time. Various SiO_x defect state of Si^{1+}, Si^{2+} and Si^{3+} are observed, which is caused by the formation of native oxide. Right: the Si 2*p* spectra as a function of sputtering time in case of oxidized Si NWs for 30 min with SiO_2 shell thickness of 28 nm. While SiO_2 peak only revealed before the sputtering, SiO_x state began to emerge with increasing sputtering time from 5 min to 20 min. After sputtering for 25 min, the SiO_2 shell was completely removed and the SiO_x state also disappeared; i.e. defect states are distributed in oxidized Si NWs from the interface between the Si core and SiO_2 shell to near the subsurface of the SiO_2 shell.

Supporting Figure S6.