Oxidation Models for Crystalline Silicon Nanowires

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Mathematical techniques for calculating the thickness of a grown oxide layer on Silicon nanowires (SiNWs) are described here. In previous publications [1,2], we showed that SiNWs, when oxidized, develop a squarish shape, as shown in Fig. 1. For the sake of simplicity, these calculations were made by using the traditional oxidation formulae developed by Deal-Grove [3] originally and improved by Massoud [4,5] for thin and ultrathin oxide layers for planar Silicon (Si).

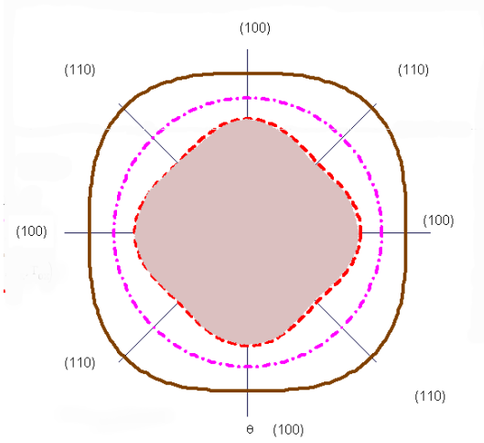

Fig. 1 Oxidization of crystalline SiNWs results in squared-up SiNWs, because (100)-oriented Si and (110)-oriented Si oxidize at different rates. In this image, the outer layer is SiO_2, and the inner layer is the unoxidized core of the SiNW.

In addition to the squaring tendency, SiNWs have a cylindrical shape to start, so that formulae based on Fick's Law for planar Si will not work well for this model. There are several methods that have been introduced over the years similar to this problem, such as the oxidation of biological tissue [6] and the freezing of ice (as a heat problem) [7].

Problems of this nature are considered to be "Stefan," or "moving boundary" problems. This is a diffusion problem, but it is primarily the diffusion of oxygen through a solid, silicon dioxide (SiO_2), with an interior moving boundary (Si converts to SiO_2 as oxygen diffuses up to the boundary and combine with Si) and a growing exterior surface (SiO_2 surface expands as the interior absorbs oxygen atoms).

References

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