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Wet and plasma-assisted oxidation of small Si nanowires at room temperature: reactive molecular dynamics study

Umedjon Khalilov[1], Erik C. Neyts[1], Geoffrey Pourtois[2], Adri C. T. van Duin[3]

[1]University of Antwerp, Antwerp, Belgium [2]IMEC, Leuven, Belgium [3]Penn State University, Pennsylvania, United States

umedjon.khalilov@ua.ac.be

During the last years, the interest in silicon nanowires (Si-NWs) has increased significantly thanks to their possible application in novel nanoscale electronic devices [1]. Small-diameter (< 10 nm) Si-NWs are also potentially very attractive with their quantum size effects, i.e., it is possibly to widen the band gap of Si-NW materials by decreasing their diameter [2]. This indicates the possibility of developing such materials with a controllable band gap. Therefore, several growth methods of small Si-NW are developed, and their growth behaviour is studied intensively. Often, thermal oxidation is used to reduce the Si-NW diameter. The growth and investigation of an oxide shell around such wires are of great importance [3].
Careful studies are needed to unravel the precise oxidation mechanisms of Si nanowires with a small diameter on the atomic scale. In this contribution, we report on both wet and plasma-assisted oxidation of a Si(100) nanowire with initial diameter of 2 nm at 300 K. The growth process of SiO_2 during thermal oxidation of Si nanowire at the atomic scale is studied by reactive molecular dynamics (MD) simulations. Forces on the atoms are derived from the ReaxFF potential [4].
Self-limiting oxidation mechanisms are discussed. Formation of SiO_2 layers are analyzed by distribution of Si-suboxide components. We found that the Si-core radius and the SiO_x ($x<2.0$) oxide shell can be precisely controlled in the nanoscale regime by controlling the type of oxidant species (O, O_2, O_3, OH, H_2O_2, NO and H_2O) at 300 K. The obtained structures are analyzed in detail.
This study is important for the fabrication of nanoscale devices in general and nanowire field-effect transistors in particular.
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Keywords
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