www.mrs.org.sg

IUMRS - ICEM2016

International Union of Materials Research Societies
- International Conference on Electronic Materials 2016

4 - 8 July 2016
SUNTEC Singapore

Organised By

Materials Research Society Singapore

In Association With

NUS National University of Singapore

Nanyang Technological University

A*STAR Singapore Agency for Science, Technology and Research

Supported by

YourSingapore

Singapore Exhibition & Convention Bureau

N-4
15 min

ICEM16-A-0375 Contributed

Oxygen Adsorption Behavior of InAs Nanowire by Ab-Initio Calculations

In Won YEU[1], Cheol Seong HWANG[2], Jung-Hae CHOI[1#+]

[1]*Korea Institute of Science and Technology (KIST), South Korea*, [2]*Seoul National University, South Korea*

[#]*Corresponding author: choijh@kist.re.kr* [+]*Presenter*

The non-planar FET device structures based on III-V compound channels are in active research interest for the sub 10 nm technology node, therefore, they demand intensive understanding and control of various factors, such as shape, size, surface and interface as well as those of bulk material properties. The stable structure of the bulk InAs is zinc-blende (ZB), while that of nanowire (NW) is wurtzite (WZ). It implies that the oxidation of the NW surfaces will be also different from that of the planar surfaces and the formation of oxide is known to be critical in the Fermi level pinning. Therefore, the investigation of the oxygen adsorption on the NW surface as an initial oxidation step is not only necessary for the theoretical understanding but also for the improvement in the device performance. In this study, the effects of diameter and the edges of InAs NWs on the adsorption of an atomic oxygen are investigated using ab-initio calculations. As models of InAs NW structure, both ZB and WZ structures are considered. For ZB NWs, either an equilateral hexagonal with {110} side walls or hexagonal with {112} sidewalls are investigated, while for WZ NWs, either an equilateral hexagonal with {11-20} side walls or hexagonal with {10-10} side walls are investigated. The adsorption energy of oxygen atom and the barrier energy for an oxygen atom to substitute a surface arsenic atom are compared for each NW surface and the corresponding planar surface to examine the effects of surface to volume ratio and existence of edges.