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Title: Micromechanism of Oxygen Transport during Initial Stage Oxidation in Si(100) Surface: A ReaxFF Molecular Dynamics Simulation Study

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PII: S0169-4332(17)30339-2
DOI: <http://dx.doi.org/doi:10.1016/j.apsusc.2017.01.302>
Reference: APSUSC 35097

To appear in: *APSUSC*

Received date: 25-9-2016
Revised date: 20-12-2016
Accepted date: 30-1-2017

Please cite this article as: Yu Sun, Yilun Liu, Xuefeng Chen, Zhi Zhai, Fei Xu, Yijun Liu, Micromechanism of Oxygen Transport during Initial Stage Oxidation in Si(100) Surface: A ReaxFF Molecular Dynamics Simulation Study, *Applied Surface Science* (2017), <http://dx.doi.org/10.1016/j.apsusc.2017.01.302>

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- A competition mechanism between thermal actuation and compressive stress blocking was found for the oxygen transport.
- At low temperature, a compressive stress was generated in the oxide layer which blocked oxygen transport into the deeper region.
- O atoms gained larger possibility to go deeper inward as temperature increase.
- The related film quality was well explained by the competition mechanism.

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