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

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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.