

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Carrier-Induced Lattice Instability in Amorphous Oxide Semiconductors YONG-SUNG KIM, HO-HYUN NAHM, Korea Research Institute of Standards and Science, DAE-HWAN KIM, Kookmin University — Amorphous oxide semiconductors (AOS's) have high electron mobility even in amorphous phase. The AOS-based thin film transistors (TFTs) are nowadays intensively pursued to be adopted into high-resolution flat-panel displays. However, a facing bottleneck of the AOS-based TFT display applications is the instability problem under bias and illumination stress conditions. Especially, by negative bias and illumination stress (NBIS) or only by illumination stress (IS), the threshold voltage of the AOS TFTs is largely negative-shifted. In this work, we study the instability mechanism of the AOS's based on first-principles calculations. The valence band tail states of the AOS's are found to be characterized by the O-O $pp\sigma^*$ anti-bonding state. The excited localized-holes thus give lattice instability and form O-O bonds through the $pp\sigma$ -hybridized interaction. The $pp\sigma^*$ level is heightened up into the conduction bands along with the O-O bond formation, and two electrons left from the created O-vacancy (V_O) occupy the delocalized conduction band states. The O-O and V_O complex (a peroxide defect) is found to be a meta-stable donor defect and suggested as an origin of the NBIS and IS instabilities in AOS TFTs. Based on the suggested mechanism, we propose a direction to improve the stability of AOS thin films with optimizing the cation compositions.

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Date submitted: 25 Nov 2012

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