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Origin of interfacial gap states in Ga_2O_3 layer grown on GaAs surface and interface passivation by F and Gd WEICHAO WANG, K. XIONG, Department of Materials Science & Engineering, The University of Texas at Dallas, ROBERT M. WALLACE, KYEONGJAE CHO, Department of Materials Science & Engineering and Department of Physics, The University of Texas at Dallas — III-V compound semiconductors are potential candidates to replace Si as the channel of future high performance n-MOSFETs. However, the poor III-V/dielectric interface quality leads to low performance of device operations. Prior to any high-k deposition on III-V, a passivated III-V surface could help to obtain a high quality high-k/III-V interface. We examine the native oxides of Ga_2O_3 on GaAs with density functional theory to determine the origin of gap states and propose possible ways to passivate the interface. Ga_2O_3 molecular species is gradually added in first principles molecular dynamics until one monolayer formed on the top of GaAs at 700 K within 3 ps. During the growth process, O atoms tend to diffuse into GaAs, and Ga-Ga dimer forms as well. The interface states originate from the Ga dangling bonds, Ga-Ga dimers and under-coordinated Ga suboxides Based on the understanding of the origin of the gap states, F and Gd are proposed to remove the gap states.

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