

Origin of gap states in GaAs/HfO₂ interface

Weichao Wang¹, Robert M. Wallace^{1,2}, and Kyeongjae Cho^{1,2,*}

¹ Department of Materials Science & Engineering and ² Department of Physics,

The University of Texas at Dallas, Richardson, TX 75080

On the demand of constantly scaling of microelectronic devices to ever smaller dimensions, SiO₂ gate dielectric was substituted with higher dielectric constant materials, Hf(Zr)O₂, to minimize current leakage through dielectric thin film. However, upon interfacing with high-K dielectrics, the electron mobility in the conventional Si channel degrades due to Coulomb scattering, surface roughness scattering, remote phonon scattering, and dielectric charge trapping. III-V is one promising candidate with superior mobility over Si. Nevertheless, Hf(Zr)O₂/III-V has much more complicated interface bonding than Si based interfaces. Successful fabrication of a high quality device depends critically on understanding and engineering of the bonding configurations at Hf(Zr)O₂/III-V interfaces. Thus, an accurate atomic insight of the interface bonding and mechanism of interface gap states formation becomes essential^{1,2,3}.

The electronic structure of the GaAs/HfO₂ interface is calculated through a hybrid density functional scheme, which produces band gaps and equilibrium lattice parameters in much better agreement with experiment than local density or generalized gradient approximations^{4,5}. 25% Hartree-Fock exchange potential was incorporated into that within Perdew-Burke-Ernzerhof (PBE)⁶ potential. Our study shows that As-As dimer bonding, Ga partial oxidation (between 3+ and 1+) and Ga- dangling bonds constitute the major contributions to gap states. These findings provide insightful guidance for interface passivation.

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