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Local dielectric constants in metal-oxide and oxide-oxide interfaces: an ab initio approach to address interfacial effects BORA LEE, CHOONG-KI LEE, SEUNGWU HAN, Ewha Womans Univ., SHANG-HO JEON, BAE-HO PARK, Konkuk Univ. — Recent experiments indicate that the dielectric constants of thin film oxides are strongly affected by interfaces formed between the oxide and metal or between different oxides. Such interfacial effects will be crucial to high-k dielectric stacks employing oxide materials with nanometer thickness. Therefore, systematic studies on interfacial effects are very important for materials selection and process design of gate stacks. In this presentation, we study on local dielectric constants in metal-oxide and oxide-oxide interfaces within the first-principles framework. Firstly, we introduce an efficient method to calculate local dielectric constants by employing slab models exposed to the vacuum. The static as well as optical dielectric constants are obtained from the change in electrostatic potentials upon the application of external electric fields. Our method can be easily adopted using conventional codes without any modification of the program. We apply this method to investigate interfacial dielectric constants in Au/MgO, Ni/ZrO2, Pt/HfO2, Ni/HfO2, Al/HfO2, SiO2/HfO2, and Al2O3/HfO2 interfaces. Our results show the presence of interfacial region with dielectric constants significantly different from that of the bulk. Microscopic explanations will be provided based on the dynamic charges and hardening/softening of phonons.

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