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Band alignment in metal-oxide interface Al/SiO_2 and Cu/SiO_2 in presence of defect JIANQIU HUANG, CELINE HIN[1], Virginia Tech, VIRGINIA TECH TEAM — Semiconductors have wide use especially in electronic devices. Technological development tends to decrease the physical size of the electronic devices into the nanoscale. Dielectric Breakdown was an old problem has never been fully resolved, which exponentially related to the size of electronic devices. It causes a severe and irreversible degradation on integrated circuits. Therefore, the motivation and main purpose of this research is to explore the dominant factors that will cause dielectric breakdown to occur in order to develop techniques to effectively prevent this occurrence. Density functional theory has been used to study the interface of Al/SiO_2 and Cu/SiO_2. Results on the investigation of atomic and charge vacancies at the interface will be presented and compared with the defect free models. The band alignment has been constructed in order to describe the behavior of the conduction band in the depletion layer. From the comparison and band alignment, a row conclusion that causes the breakdown occurrence was made.

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