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Density Functional Theory Study of Silicon Chlorides for Atomic Layer Deposition of Silicon Nitride Thin Films

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Recently, the scaling of conventional planar NAND flash devices is facing its limits by decreasing numbers of electron stored in the floating gate and increasing difficulties in patterning. Three-dimensional vertical NAND devices have been proposed to overcome these issues. Atomic layer deposition (ALD) is the most promising method to deposit charge trap layer of vertical NAND devices, SiN, with excellent quality due to not only its self-limiting growth characteristics but also low process temperature. ALD of silicon nitride were studied using NH3 and silicon chloride precursors, such as SiCl4[1], SiH2Cl2[2], Si2Cl6[3], and Si3Cl8. However, the reaction mechanism of ALD silicon nitride process was rarely reported. In the present study, we used density functional theory (DFT) method to calculate the reaction of silicon chloride precursors with a silicon nitride surface. DFT is a quantum mechanical modeling method to investigate the electronic structure of many-body systems, in particular atoms, molecules, and the condensed phases. The bond dissociation energy of each precursor was calculated and compared with each other. The different reactivities of silicon chlorides precursors were discussed using the calculated results.

Keywords: Density functional theory, Atomic layer depostion, Silicon chlorides, Silicon nitride

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Non-volatile Control of 2DEG Conductance at Oxide Interfaces

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Epitaxial complex oxide thin film heterostructures have attracted a great attention for their multifunctional properties, such as ferroelectricity, and ferromagnetism. Two dimensional electron gas (2DEG) confined at the interface between two insulating perovskite oxides such as LaAlO3/SrTiO3 interface, provides opportunities to expand various electronic and memory devices in nano-scale. Recently, it was reported that the conductivity of 2DEG could be controlled by external electric field. However, the switched conductivity of 2DEG was not stable with time, resulting in relaxation due to the reaction between charged surface on LaAlO3 layer and atmospheric conditions. In this report, we demonstrated a way to control the conductivity of 2DEG in non-volatile way integrating ferroelectric materials into LAO/STO heterostructure. We fabricated epitaxial Pb(Zr0.2Ti0.8)O3 films on LAO/ STO heterostructure by pulsed laser deposition. The conductivity of 2DEG was reproducibly controlled with 3-order magnitude by switching the spontaneous polarization of PZT layer. The controlled conductivity was stable with time without relaxation over 60 hours. This is also consistent with robust polarization state of PZT layer confirmed by piezoresponse force microscopy. This work demonstrates a model system to combine ferroelectric material and 2DEG, which guides a way to realize novel multifunctional electronic devices.

Keywords: two-dimensional electron gases, ferroelectric, non-volatile memory