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Understanding The Ferroelectric $Hf_{0.5}Zr_{0.5}O_2$ formation Based on Kinetic Model

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Abstract

$Hf_{1-x}Zr_xO_2$ (HZO) is a kind of ferroelectric (FE) material that holds promise for transistors and non-volatile memory due to great compatibility to CMOS technology. Although current studies support the importance of this material, the efficiency of ferroelectric formation limits HZO towards being fully engaged to the desired technologies. In this study, the kinetic model would predict the phase formation and phase transition of HZO film which has three phases of the orthorhombic (*O*), tetragonal (*T*) and monoclinic (*M*) phases. It is able to predict the condition of crystallization and phase transition during the thermal rapid and cooling process that govern ferroelectricity in HZO thin film. Our simulation reveal that the comparable interfacial energy between capping electrode and HZO would suppress the *M*-phase formation and enable more phase transition from *T*- to *O*-phase. By incorporating the kinetic model into the results from XAS mapping technique, we propose a soak annealing process to optimize the ferroelectric HZO. The process enabled HZO with a polarization (P_s) value up 64.52 μC cm^{-2}, which is the largest P_s ever reported in HZO system. The significant ferroelectric enhancement with soak annealing is due to the effective $T \rightarrow O$ phase transition along with the *M*-phase suppression.