

Abstract Submitted  
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**Theoretical study of the atomic structure and thermodynamics of amorphous hafnia** XUHUI LUO, UT Ausitn, ALEX DEMKOV, UT Austin — Hafnium dioxide is now used in Si technology and is considered a possible gate dielectric in III-V channel devices. As deposited,  $\text{HfO}_2$  films are disordered, however, the low temperature of crystallization is an obstacle to further scaling. Thus understanding the thermodynamic properties of amorphous hafnia is of great importance. Owing to extremely high melting temperature there are rather few experimental studies of amorphous hafnia quenched from the melt. This makes a theoretical study rather attractive. We use first principles melt-quench procedure to generate theoretically atomistic models of amorphous hafnia. We find that there are two types of amorphous structures. Type I amorphous structures (related to tetragonal hafnia) have molar volume between that of monoclinic and tetragonal hafnia. The energy is  $0.30 \text{ eV}/(\text{HfO}_2)$  higher than that of the monoclinic phase. The volume of type II amorphous hafnia (related to monoclinic hafnia) is about 4% larger than that of monoclinic hafnia. This is comparable to that of the disordered films grown by atomic layer deposition (ALD). The energy of type II amorphous structure is  $0.60 \text{ eV}/(\text{HfO}_2)$  above that of the monoclinic phase. We use the nudged elastic band method to calculate the transition barrier between the monoclinic phase and type II amorphous hafnia. The calculated barrier of  $0.15 \text{ eV}/(\text{HfO}_2)$  suggests the crystallization temperature of about 900K which is close to experiment.

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