Structural properties and electronic structures of amorphous HfO\(_2\)/Si(001) interface

CHEN GUOHONG, HOU ZHUFENG, GONG XINGAO, Surface Physics Laboratory and Department of Physics, Shanghai-200433, XG-GONG’S GROUP TEAM — Using the projector augmented wave method within the generalized gradient approximation, we have performed *ab-initio* molecular dynamics simulations to generate an atomic structure model of amorphous hafnium dioxide (\(a\)-HfO\(_2\)) by a melt-and-quench scheme, and have investigated the structural and electronic properties of \(a\)-HfO\(_2\)/Si(001)-(2\(\times\)2) interface. The structure of \(a\)-HfO\(_2\) sample is analyzed via atomic coordination number and partial pair-radius distribution functions. Our results show the average Hf-O nearest-neighbor distance is 2.06 \(\AA\), which is comparable with the Hf-O bond lengths (in the range from 2.04\(\sim\) to 2.25\(\sim\)) in monoclinic HfO\(_2\) crystalline, and also indicate the generated sample essentially reflects the experimentally measured structural characteristics of \(a\)-HfO\(_2\). Most importantly, it is found that the valence band offset of \(a\)-HfO\(_2\)/Si interface is about 2.97\(eV\), and our results suggest that the coordination of Si atoms at interface would significantly affect the electronic properties of interface.

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