Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Effect of oxygen vacancies and strain on the phonon spectrum of HfO_2 LINGYUAN GAO, Univ of Texas, Austin, EILAM YALON, ANNABEL CHEW, ERIC POP, Stanford University, ALEX DEMKOV, Univ of Texas, Austin, DEPARTMENT OF MATERIALS SCIENCE AND ENGINEERING, STANFORD UNIVERSITY TEAM, DEPARTMENT OF ELECTRICAL ENGINEERING, STANFORD UNIVERSITY TEAM, DEPARTMENT OF PHYSICS, UNIV OF TEXAS, AUSTIN TEAM — The effect of strain and oxygen deficiency on the Raman spectrum of monoclinic HfO_2 is investigated theoretically using first-principle calculations. In-plane compressive strain is found to blue shift the phonon frequencies, while tensile strain does the opposite. The simulations are compared to and good agreement is found with experimental results of Raman frequencies greater than 110 cm^{-1}. Several Raman modes measured below 110 cm^{-1} and previously assigned to HfO_2 cannot be assigned to HfO_2. However, localized vibrational modes introduced by threefold-coordinated oxygen (O_3) vacancies are identified at 96.4 cm^{-1} These results are important for a deeper understanding of vibrational modes in HfO_2, which has technological applications in transistors, and particularly in resistive random-access memory (RRAM) whose operation relies on oxygen-deficient HfO_x

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Date submitted: 12 Nov 2016 Electronic form version 1.4