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# Ab initio study of the electronic structure and the EFG at Ta sites in HfO2:Ta y ZrO2:Ta.

text

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## Summary

Hafnia (HfO2) and zirconia (ZrO2) are wide band gap semiconductors with high dielectric constants and very similar properties. Both oxides have monoclinic structure at room temperature that transforms into tetragonal and cubic at respectively higher temperatures. Besides both oxides display technological interest because their high temperature melting point as well as its chemical stability.
By adding small amounts of impurities present different structures that have important technological applications such as electrolytes for combustion cells, catalytic substrates and protecting coatings.
Both, HfO2 and ZrO2 have been widely studied using Time Differential Perturbed Angular Correlations spectroscopy (TDPAC) using 181Hf→181Ta probes. Up to now the analysis of TDPAC results was based in the simple assumption that probes are inert in the sense that they do not introduce any crystalline or electronic distortion.
In this contribution we present a first principles study (using the full-potential linear augmented plane wave plus local orbital, APW+lo) of structural, electronic and hyperfine properties of Ta impurities localized at cationic sites in monoclinic HfO2 and ZrO2. Due to the agreement between the experimental results obtained by TDPAC and our calculations of the electric field gradient tensor (EFG) it was possible to deduce the Ta charge state at 300K. It was also possible to calculate the structural distortions induced by the impurities in both oxides. From these results the role played by the Ta impurity to create the EFG can be determined.

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