Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

First principles MD simulations of proton diffusion in cubic perovskite $BaZrO_3$ MARCO FRONZI, YOSHITAKA TATEYAMA, National Institute for Material Science, NICOLA MARZARI, École Polytechnique Fédérale de Lausanne, ENRICO TRAVERSA, National Institute for Material Science — The development of highly proton conductive and chemically stable ceramic materials, including doped barium zirconate, is particularly important for the fabrication of high performance solid oxide fuel cell (SOFCs) operating at intermediate-low temperature (550-900K). In this work, extensive first-principles molecular dynamics simulations have been employed to analyze proton self-diffusion in cubic perovskites BaZrO3. Simulations have been performed at 1300K, that are typical fuel-cells' working conditions. The runs were carried out for the stoichiometric system in unit cells of 40 atoms, and in the canonical ensemble. We also studied the effect of applied compressive and tensile stresses on the proton motion finding a non linear effect on the proton mobility as a function of the stain. Enhanced diffusion has been found for an isotropic compression of 2% in the lattice parameter. On the other hand, the presence of a tensile strain does not seem to affect the proton diffusion, compared to the equilibrium case. The power spectrum obtained by the velocity-velocity correlation function for the proton shows no significant change in the vibrational frequencies for the strains studied.

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Date submitted: 07 Dec 2011 Electronic form version 1.4