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Oxygen vacancy effect on dielectric and hysteretic properties of zigzag ferroelectric iron dioxide nanoribbon

S. Zriouel^{1,2,*}, B. Taychour², F. El Yahyaoui², L.B. Drissi^{2,3,†}

1- Department of Physics, Polydisciplinary Faculty,

Sultan Moulay Slimane University in Beni Mellal, Morocco

2- Lab-PHE, Modeling & Simulations, Faculty of Science, Mohammed V University, Rabat, Morocco

3- CPM, Centre of Physics and Mathematics, Faculty of Science,

Mohammed V University, Rabat, Morocco and

* Corresponding author: * sanae.zriouel@usms.ma

† ldrissi@fsr.ac.ma

Abstract

Zigzag FeO_2 nanoribbon defected by the removal of oxygen atoms is simulated using Monte Carlo simulations. All possible arrangements of positions and number of oxygen vacancy are investigated. Temperature dependence of polarization, dielectric susceptibility, internal energy, specific heat and dielectric hysteresis loops are all studied. Results show the presence of second order phase transition and Q-type behavior. Dielectric properties dependence on ribbon's edge, positions and number of oxygen vacancy are discussed in detail. Moreover, single and square hysteresis loops are observed whatever the number of oxygen vacancy in the system.

Keywords: Monte Carlo simulations; FeO2 materials; Oxygen vacancy; hysteresis loops; polarization; dielectric susceptibility; critical temperature; RKKY interaction.

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