Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Electron Energy Structure and Electron Paramagnetic Resonance of Binuclear Niobium Molecules in Li-Nb Phosphate Glass Dielectrics SABRINA ARRINGTON-PEET, RAKHIM RAKHIMOV, VLADIMIR GAVRILENKO, Center for Materials Research, Norfolk State University, Norfolk VA 23504 — Electron paramagnetic resonance (EPR) spectra of Nb4+ ions in lithium-niobium phosphate glass insulators with different composition of oxide components have been studied. The EPR data reveal formation of triplet Nb binuclear complex in Li-Nb glass dielectric. Equilibrium atomic geometries of a model molecule $(OH)_3$-Nb-O-Nb-$(OH)_3$ embedded into Li-Nb phosphate glass are determined by molecular dynamics. The total energy and electron energy structure of the system have been studied by first principles generalized gradient approximation (GGA) method within density functional theory (DFT). Molecular geometry in substantially distorted as a result of external potential of the glass. Total energy analysis of the $(OH)_3$-Nb-O-Nb-$(OH)_3$ molecule embedded into Li-Nb phosphate glass indicates appearance of two non-equivalent atomic geometries with the oxygen atom in –Nb-O-Nb- fragment shifted from its undisturbed symmetrical position. Predicted modifications of electron energy structure of the system are discussed in comparison with measured EPR data.

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Date submitted: 30 Nov 2004 Electronic form version 1.4