Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Structural, dynamic and electronic properties of amorphous Al_2O_3: ab–initio molecular dynamics calculations[1] GONZALO GUTIERREZ, University of Chile, Chile, SERGIO DAVIS, Royal Institute of Technology, Sweden — First principles molecular dynamics (MD) calculations of amorphous Al_2O_3 in a system consisting of a supercell of 80 atoms is reported. A detailed analysis of the interatomic correlations allows us to conclude that the short range order is mainly composed by AlO_4 tetrahedra, but in contrast to classical MD results, also an important number of AlO_5 units are present. The vibrational density of state, calculated by means of the velocity autocorrelation function, present two main bands, a low frequency one related to the inter-tetrahedron vibration and a high frequency band related to the intra-tetrahedron vibration. By means of a geometry relaxation we obtain a fully relaxed system, and calculated its elastic properties. The reported bulk modulus is 193.4 GPa, the smallest among the several phases of alumina. The electronic properties were characterized by means of both the total and partial electronic density of states as well as by means of the electron localization function. The system present a rather small gap of 2.4 eV. The consequences of these results will be discussed.

[1]Grant Anillo ACT/24-Chile.

Gonzalo Gutierrez
University of Chile, Chile

Date submitted: 03 Dec 2007 Electronic form version 1.4