



## Computer simulations study of amorphous compounds

Gonzalo Gutiérrez, Eduardo Menéndez, Claudia Loyola, Joaquín Peralta

Departamento de Física, Facultad de Ciencias, Universidad de Chile,  
Casilla 653, Santiago, CHILE. E-mail: gonzalo@fisica.ciencias.uchile.cl

In this talk we will present molecular dynamic simulations, both classical and ab-initio, of amorphous  $\text{Al}_2\text{O}_3$  (alumina),  $\text{GeO}_2$  (germania) and  $\text{CdTeO}$  compounds, contrasting the results to their crystalline phases. We focus our attention on the structural, vibrational and electronic properties, giving an atomic description of the short and intermediate range order.

In the case of alumina, first principles molecular dynamics (MD) calculations of amorphous  $\text{Al}_2\text{O}_3$  in a system consisting of a supercell of 80 atoms is reported. A detailed analysis of the inter-atomic correlations allows us to conclude that the short range order is mainly composed by  $\text{AlO}_4$  tetrahedron, but in contrast to classical MD results, also an important number of  $\text{AlO}_5$  units are present. The vibrational density of states, obtained as a Fourier transform of the velocity autocorrelation function, presents two main bands, a low frequency one related to the inter-tetrahedron vibration and a high frequency band related to the intra-tetrahedron vibration. This vibrational density of states is compared to the one of the  $\gamma\text{-Al}_2\text{O}_3$ . The electronic properties were characterized by means of both the total and partial electronic density of states, presenting a rather small gap of 2.4 eV.

Amorphous germanium oxide ( $\text{GeO}_2$ ), a structural and chemical analog to silica ( $\text{SiO}_2$ ), is an example of covalent glass, and a good empirical pairwise inter-atomic potential to be used in computer simulation exist. In order to investigate the structural transformation under pressure, we perform MD simulations in the microcanonical ensemble, with systems at densities ranging from 3.6 to 6.3  $\text{g/cm}^3$ . The network topology of our system is analyzed through partial pair correlations, coordination number and angle distributions, whereas the vibrational properties were characterized by means of the density of states. At normal density, a detailed analysis of the inter-atomic distances reveals that in the amorphous state there is a short-range order dominated by a slightly distorted ( $\text{GeO}_4$ ) tetrahedron. Beyond that, there is an intermediate range order composed by vertex-sharing tetrahedron. The vibrational density of states has two bands, a low frequency one up to 20 [THz], and a high frequency band from 20 to 30 [THz]. According to density increases, there is a structured transformation, from a short-range order defined by the basic tetrahedron ( $\text{GeO}_4$ ) to a basic octahedron ( $\text{GeO}_6$ ). Consistent to this picture, the vibrational density of states also presents big changes, where the low frequency band shrinks, and the high frequency becomes wider and flatter.

Finally, we present an ab initio molecular dynamics calculation for the complex ternary material  $\text{CdTeO}_3$ . Amorphous thin films have been grown by means of r.f. sputtering during the last decade. In this work we predict the short range order of this compound compare it to the crystalline counterpart. The inter-atomic forces have been calculated using a plane wave pseudopotential implementation of density functional theory (Quantum-espresso). The MD simulations were conducted in the microcanonical ensemble using the Berenden's algorithm to keep the systems with the desired temperature. The samples were obtained by heating the system to 3000 K, and after equilibration, the velocity is scaled to drive the systems to 300 K. The compound is characterized using pair and angular distribution functions, coordination numbers and a description of the molecular units of the compound.

This work has been supported by grant Anillo "Computer simulation lab of nano-bio systems" ACT24/2006-Chile. We thank our collaborators Paolo Gianozzi and Sergio Davis. We also acknowledge computer time from different institutions: CINECA-Italy, the Abdus Salam International Centre for Theoretical Physics ITCP-Trieste, the Center of Bioinformatics and Molecular Simulation of the University of Talca-Chile, and MAIDROC Computer Lab and CESMEC, both from Florida International University-Miami.