Structural and vibrational properties of amorphous GeO_2 under pressure: a molecular dynamics study.

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We studied the structural and dynamical properties of amorphous germanium oxide (GeO_2) by means of the molecular dynamics technique. The simulations were done in the micro-canonical ensemble, with systems at densities ranging from 3.6 to 6.3 g/cm^3, using a pairwise potential. The network topology of our system is analyzed through partial pair correlations, coordination number and angle distributions. The vibrational properties were characterized by means of the density of states, obtained as a Fourier transform of the velocity autocorrelation function.

At normal density [1], 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 (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], related to the inter-tetrahedra vibration and a high frequency band from 20 to 30 [THz] related to the intra-tetrahedron vibration.

According to density increases, there is a structural transformation, from a short-range order defined by a building block composed by a basic (GeO_4) tetrahedron **Fig. 1** to a basic (GeO_6) octahedron **Fig. 2**, which implies a large change in density and in the short and medium range order [2]. 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.

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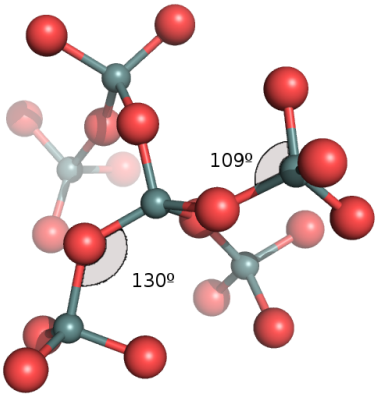

Fig. 1 *GeO_2 at normal pressure.*

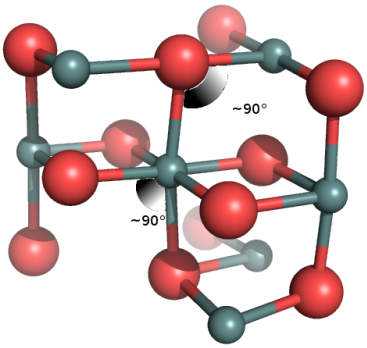

Fig. 2 *GeO_2 at high pressure.*

References

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