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Structural Study of β-TeO_3 : Raman Spectrum Interpretation by Quantum Chemistry

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The TeO_3-based materials are particularly promising as a challenge in the research and elaboration of new microwave dielectric materials for Low Temperature Cofired Ceramics (LTCC) technology [1, 2]. The LTCC process allows the integration and the miniaturization of passive electronic components in functional three-dimensional devices.

To improve the properties of these materials it is necessary to control and manage their synthesis and to better understand their peculiar crystal chemistry.

This communication presents the results obtained on the simplest TeO_3-based material, called β-TeO_3. It was synthesized by oxydation of the stable α-TeO_2 phase and studied by both X-ray diffraction and Raman scattering techniques. The bands in the Raman spectra were first interpreted on the basis of lattice dynamical model treatments but some of them, in the high frequency region, could not be attributed with precision. Quantum chemistry has thus been used to circumvent this problem, in the framework of density functional theory (CRYSTAL06 program), and allowed to elucidate the whole spectrum as it will be explained on the poster.

The Raman study of the β-TeO_3 structure confirms the three-dimensional character of the edges-sharing [TeO_6] regular octahedra stackin. Those octahedra are the fingerprint of tellurate compounds, *i.e.* oxides containing Te^{VI} although only β-TeO_3 possesses them regular. In the other tellurium-based oxide family, the tellurites (containing Te^{IV}), the building block is an irregular [TeO_4] disphenoid.

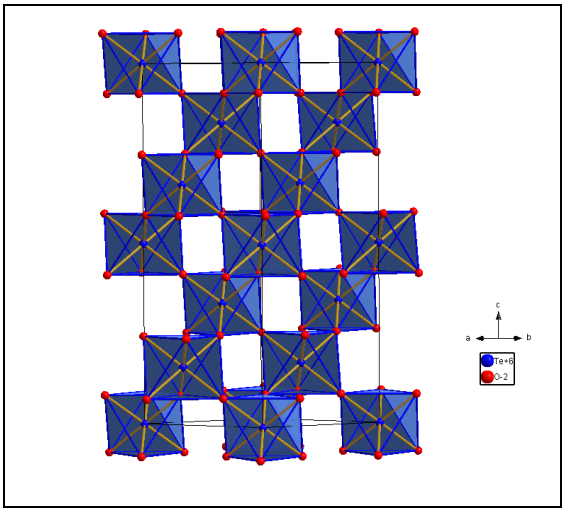

Figure 1: Structure of β-TeO_3 [3]

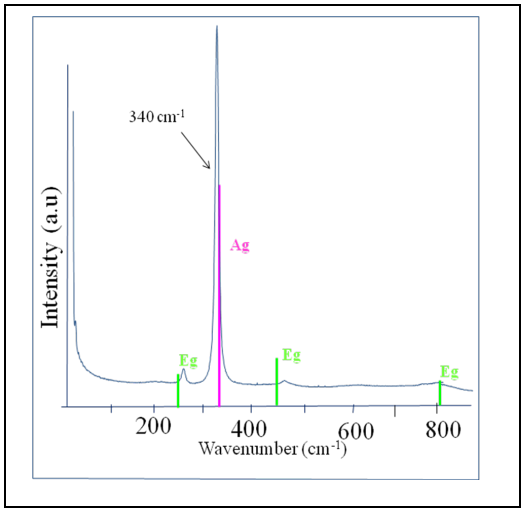

Figure 2: *Raman spectra experimental and modeling of β-TeO_3*

References

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[3] M.Dusek, J.Loub, Powder Diffraction, Vol. 3, No. 3, September 1988