Atomistic Simulations of TeO$_2$-based Glasses: Interatomic Potentials and Molecular Dynamics

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TeO$_2$-based materials are remarkable from fundamental and engineering points of view. In particular, the TeO$_2$-based glasses appear to be among the most interesting materials for nonlinear optoelectronic devices. Their nonlinear susceptibilities are the highest among the known oxide glasses. The origin of this property partly relates to the lone electron pair (LP) of tellurium atom which is stereo-chemically active and is responsible for peculiarities in the short-range atomic arrangement. Description of the glass structure is the first step towards understanding its properties.

Investigations of the glass structure by means of molecular dynamics (MD) methods require establishing the interatomic potentials (IAP) for Te-O system. While glasses lack the long-range order characteristics of crystals, the chemical forces controlling the short-range order are similar. Therefore, knowledge of local structure in various crystalline compounds can clarify the Te$^{IV}$ atom environment in glasses. We developed IAPs that are able to reproduce cell parameters and various tellurium atom environments (from TeO$_3$ to TeO$_6$ structure units) of number of TeO$_2$ polymorphs and tellurite compounds. Our model takes into account polarization effect for oxygen ions and effect of the presence of the 5s$^2$ LP around tellurium atoms by presenting core-shell model for both atom species.

We applied our potentials to the MD study of pure TeO$_2$ glass and obtained a good agreement of calculated pair distribution function with experimental one. From the results of MD simulations we obtained the information about short- and medium-range order in the glass structure as bond-angle distribution, coordination of atoms, forming structural units and their interconnection.