AB-INITIO MOLECULAR DYNAMICS SIMULATIONS OF THE STRUCTURE OF LIQUID ALUMINATES

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Over the past few years an increasing number of works devoted to structural studies of molten materials have been carried out thanks to the development of containerless methods. These techniques have created new opportunities to study high-temperature liquids with a very high degree of control. The CRMHT in Orleans (France) has chosen to combine aerodynamic levitation with CO_2 laser heating and has developed various apparatus to combine these techniques with x-ray and neutron diffraction at synchrotron and neutron sources [1-3].

It is not always obvious to determine precise structural models from the experimental data. In fact, because of the absence of long range order, the experiments can give only a partial and incomplete description of the atomic structure of the molten liquids (interatomic distances and a number of neighbors). In particular, the structural studies of complex materials are often difficult. One of the difficulties arises from the fact that the measured structure factor S(Q) and the corresponding pair correlation function g(r) are weighted sums of the partial functions for the different atom pairs and sometimes various structural models can be consistent with the experimental results. Thus, the coupling of experimental and simulation techniques becomes essential for defining structural models consistent with all the available experimental data.

We have investigated the structure of liquid $Y_3Al_5O_{12}$ (YAG) above its melting point (mp=2220K) by using x-ray and neutron scattering. *Ab-Initio* Molecular Dynamics (AIMD) simulations were carried out using the VASP code [4] where the interatomic forces are obtained from density functional theory. Experimental and simulation results will be compared. Results obtained with other aluminates will be also presented.

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