
Developing interaction potentials for modelling oxide glasses

Siddharth Sundararaman^{1,2}, Liping Huang¹, Simona Ispas^{*2}, and Walter Kob²

¹Department of Materials Science and Engineering, Rensselaer Polytechnic Institute – Troy, NY 12180, United States

²Laboratoire Charles Coulomb (L2C) – Univ. Montpellier, Univ. Montpellier, CNRS – Montpellier, France

Abstract

We propose a new scheme to parametrize effective pair potentials that can be used to simulate oxide glasses. As input data for the optimization we use the radial distribution functions of the liquid and the vibrational density of state of the glass, both obtained from ab initio simulations, as well as experimental data on the pressure and/or composition dependence of the density and the elastic moduli of the glass [1].

For the case of silica we find that this new scheme allows to find potentials that are significantly accurate than previous ones even if the functional form is the same, thus demonstrating that even simple two-body potentials can be superior to more complex three-body potentials. We have tested the new potential by calculating the pressure dependence of the elastic moduli and find a good agreement with the corresponding experimental data.

For binary alkali (lithium, sodium, potassium) silicate glasses, the new potentials allow to reproduce the composition dependence of both density and elastic moduli. Further, we examine the capabilities of these potentials for studying ternary compositions containing two alkali oxides, and we find that they are reliable even if they have been developed for binary compositions.

Simplicity of the functional form also makes these potentials computationally more efficient than potentials with more complex functional forms, and hence more suitable for simulations involving large length and/or time scales.

S. Sundararaman, L. Huang, S. Ispas, and W. Kob, "New optimization scheme to obtain interaction potentials for oxide glasses", to be submitted (2017)

Keywords: atomistic simulation, oxide glasses, interaction potential, fitting scheme, mechanical properties

*Speaker