ID: 1.1.1b

Title: Ab initio molecular dynamics study of diffusion mechanism in liquid B_2O_3 under pressure

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Computer simulation based on molecular dynamics is powerful approach to clarify the microscopic mechanism of atomic diffusion in liquid state under pressure. Transport properties of covalent liquids under pressure are very interesting in the sense that they show unexpected pressure dependence. For a number of covalent liquids, such as SiO$_2$ and B$_2$O$_3$ abnormal behaviour of the viscosity has been observed, i.e. the viscosity significantly drops with pressure. This anomalous behaviour of the viscosity is considered to be related to the atomic diffusion in the liquids under pressure. It is, however, unclear how the rearrangement process of the covalent bonds is affected by compression. In order to explore the pressure dependence of microscopic diffusion mechanism in covalent liquids, we performed {\em ab initio} molecular dynamics simulations for liquid B$_2$O$_3$ which is a typical covalent liquid. From our calculation, two interesting properties about pressure dependence of diffusion coefficients are found. One is that diffusion coefficients of liquid B$_2$O$_3$ increase despite increasing pressure up to 10 GPa. The other is that the diffusivity of O atoms is reduced more quickly than that of B atoms with compression above 10 GPa. Our molecular dynamics simulation successfully reveals the microscopic origin of these anomalous pressure dependence of diffusivity. Around 10 GPa, covalent bonds are always exchanged by concerted reaction while the non-bridging oxygens (NBO) are needed for atomic diffusion at ambient perssure. These facts suggest that the atomic diffusion with concerted reaction gives the diffusion maximum. At about 100 GPa, 2/3 O atoms are overcoordinated to B atoms while almost all B atoms are overcoordinated to O atoms. This asymmetry property gives rise to difference in the pressure dependence of the diffusivity. In our presentation, we discuss the details of the pressure dependence of microscopic diffusion mechanism in liquid B$_2$O$_3$.