Ab initio molecular dynamics study of atomic diffusion in covalent liquid under high pressure

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Transport properties of covalent liquids under high pressure are very interesting in the sense that they show unexpected pressure dependence. For a number of covalent liquids, such as SiO_2, B_2O_3 and silicates abnormal behavior of the viscosity has been observed, i.e. the viscosity significantly drops with increasing pressure [1, 2, 3]. This anomalous behavior 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 *ab initio* molecular dynamics simulations for liquid B_2O_3 and liquid basaltic aluminosilicate. These liquids has diffusivity maximum (viscosity minimum) under high pressure. We investigate the microscopic diffusion mechanism under high pressure. In the presentation, we discuss the origin of the anomalous pressure response of diffusivity from microscopic point of view.

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