Structural change of liquid sulfur from polymeric liquid to simple liquid under high pressures

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Liquid sulfur consists of S8 ring molecules near the melting temperature of 388 K. With increasing temperature, a structural transition from molecular liquid to chain polymeric liquid occurs. For high pressure conditions, some experimental and theoretical studies have been reported [Brazhkin 1991; Zhao, 2014; Liu, 2014; Plašienka, 2015] for structural changes in liquid sulfur from long-chain to short-chain structures under high pressure up to 15.8 GPa. However, structural properties under further high pressure (*i.e.,* structures that reach beyond a chain structure) have not been discussed. For this reason, in this study, we have investigated the structural properties of liquid sulfur under high pressures up to approximately 500 GPa by means of *ab initio* molecular dynamics simulations. From our simulations, it is found that the liquid sulfur has a covalent-like interactions even in metallic state, and liquid sulfur has a simple liquid structure at 320 GPa and higher pressures [Ohmura 2019]. In this study, we will also discuss the similarities of pressure-induced structural change in other liquid chalcogens[Shimojo, 2003; Ohmura, 2011].

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