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Structure and dynamics of supercooled liquid silicon under pressure: A first-principles molecular-dynamics study. TETSUYA MORISHITA, Research Institute for Computational Sciences, National Institute AIST — Recent investigations have suggested that silicon (Si) may exhibit liquid-liquid transitions under pressure and/or supercooling [1]. Here, we report first-principles molecular-dynamics simulations of supercooled liquid Si focusing on the pressure dependence of structure and dynamics [2]. The pair correlation function of deeply supercooled liquid Si (1100 K) for pressures 0 - 18 GPa shows considerable structural changes resulting from the collapse of tetrahedral configurations. The power spectrum of the velocity auto-correlation function also confirms the reduction of the tetrahedral order by pressurization. The self-diffusion coefficient as a function of pressure shows a broad maximum around 10 GPa. However, at a higher temperature (1500 K), the diffusion coefficient simply decreases with increasing pressure, indicating conspicuous dependence of the dynamics and relevant structure upon temperature. [1] T. Morishita, Phys. Rev. Lett. 93, 055503 (2004); ibid. 97, 165502 (2006). [2] T. Morishita, Phys. Rev. E 72, 021201 (2005).

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