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Effects of pressure on transitions between disordered phases in supercooled liquid Si[1] ALEX ANTONELLI, KARL GARCEZ, Universidade Estadual de Campinas — In the last 20 years, there has been an increasing interest in liquid-liquid transitions. Substances that exhibit negative melting slopes are considered to undergo such transitions. In this work, we study the pressure effects on the transitions between the disordered phases in supercooled liquid Si through Monte Carlo simulations and efficient methods to compute free energies. Our calculations, using a realistic interatomic potential for Si, indicate that at zero pressure the liquid-liquid phase transition, between the high density liquid and the low density liquid, occurs at a temperature 325 K below melting. We found that the liquid-liquid transition temperature decreases with increasing pressure, following the liquid-solid coexistence curve. As pressure increases, the liquid-liquid coexistence curve approaches the region where the glass transition between the low density liquid and the low density amorphous takes place. Above 5 GPa, our calculations show that the liquid-liquid transition is suppressed by the glassy dynamics of the system. We also found that above 5 GPa, the glass transition temperature is lower than that at lower pressures, suggesting that under these conditions the glass transition occurs between the high density liquid and the high density amorphous.

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