Pressure-induced structural change in liquid GaIn eutectic alloy

Synchrotron x-ray diffraction reveals a pressure induced crystallization at about 3.4 GPa and a polymorphic transition near 10.3 GPa when compressed a liquid GaIn eutectic alloy up to ~13 GPa at room temperature in a diamond anvil cell. Upon decompression, the high pressure crystalline phase remains almost unchanged until it transforms to the liquid state at around 2.3 GPa. The ab initio molecular dynamics calculations can reproduce the low pressure crystallization and give some hints on the understanding of the transition between the liquid and the crystalline phase on the atomic level. The calculated pair correlation function g(r) shows a non-uniform contraction reflected by the different compressibility between the short (1st shell) and the intermediate (2nd to 4th shells). It is concluded that the pressure-induced liquid-crystalline phase transformation likely arises from the changes in local atomic packing of the nearest neighbors as well as electronic structures at the transition pressure.

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