Structure of Ge-Sb-Te liquids from Car-Parrinello molecular dynamics simulations and neutron scattering measurements

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We investigate structural and vibrational properties of four ternary compositions $Ge_6Sb_6Te_{88}$, $Ge_{10}Sb_{10}Te_{80}$, $Ge_{14}Sb_{14}Te_{72}$ and $Ge_2Sb_2Te_5$ in the liquid state. The structural properties are radial distribution functions, structure factors, coordination numbers, angular, neighbors and rings distributions. We found an excellent agreement when we compare directly the structure factors obtained in the simulations with the ones obtained experimentally using neutron scattering. We argue that this excellent agreement comes from the incorporation of dispersion forces in the simulations. The vibrational properties illustrated by the vibrational density of states are also computed and compared to the experimental data.