

Ab-initio molecular dynamics study of the pressure dependence of the collective excitations in liquid Ga-Sb alloy

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Transverse and longitudinal dynamic structures of liquid equiatomic Ga-Sb alloy are computed from ab-initio molecular dynamics simulations. Thermodynamic states ranging from ambient pressure up to 10 GPa are considered, following the melting line.

The evolution of collective dynamic properties as a function of pressure is studied in connection with the topological and chemical order. We focus on the collective propagating modes from which sound speed and shear viscosity are deduced. The issue of a possible coupling between longitudinal and transverse modes is discussed. Special attention is paid to the evolution when undergoing the liquid-liquid transition at about 4 GPa [1].

[1] D. Martinez-Garcia, Y. Le Godec, G. Syfosse, and J.P. Iti, *phys. stat. sol. (b)* **211**, 475 (1999).