Polymorphism in Fluid Phosphorus: a Joint Study of Structure and Dynamics

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The study of polymorphism in the fluid phase of single component systems is recently attracting much attention after the direct observation, by X-ray diffraction, of a first-order phase transition in liquid phosphorus at 1000 °C and 1 GPa [1].
A further study of the interesting case of phosphorus is here reported, aiming at the characterization of the structural and dynamical changes across the first-order transition with diffraction (XRD) and inelastic X-ray scattering (IXS) experiments, respectively.

The XRD experiment [2,3] has been performed on a large thermodynamic range, thus allowing us to follow the transition line up to 2200 °C at 0.3 GPa. From the shape of the transition line, a thermodynamic characterization of the transition is obtained in terms of latent heat and internal energy change. Moreover, the addition of the high-pressure high-temperature data to the known phase diagram of phosphorus allows us to conclude that this first order transition actually occurs in the fluid phase.
The IXS experiment [4] has been performed on a large exchanged momentum, q, range comprised between 2 and 13 A^{-1}. For q values up to 4.3 A^{-1}, the spectral intensities of the two fluids can be interpreted in terms of their different vibrational dynamics. At higher q, however, the spectral intensities of the two fluids become more and more similar, thus suggesting that they have indeed a very similar local structure.
These structural and dynamics studies, together with the thermodynamic characterization of the transition, give us hints to better understand the nature of this unusual abrupt transition in fluid phosphorus.

References

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