Structural and electronic properties of InSe liquids: a combined XRD, EXAFS and AIMD study

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Most of the solid semiconductors (e.g. Goup IV elements, III-V alloys) become metals when melted. However, III-VI alloys such as InSe (GaSe…) belong to these rather less common systems which do remain good semiconductors in their liquid phase (close to the melting point).
InSe crystallizes at ambient conditions in a layered phase characterized by a low average coordination (III-VI systems do obey the so-called 'octet rule'). At high pressure (~10 GPa), it undergoes a transition towards the NaCl (cubic) phase and becomes a metal [1].
These features render III-VI liquids interesting candidates for the observation of liquid-liquid transitions. Here, we shall report the results of an extensive study of the electronic and structural properties of the InSe system [1,2,3,4].
Owing to the combination of x-ray diffraction (XRD) and x-ray absorption (EXAFS) experiments, the InSe phase diagram has been determined up to 3 GPa and 1500 K [2]. This allows to measure the melting line and to evidence a solid-solid transition prior to melting. By combining *ab-initio* molecular dynamics (AIMD) simulations with EXAFS, the structure of the liquid phase close to the melting point has been determined [3]: it is shown to be made of InSe tetrahedral-like units. This low coordination character is responsible for the liquid semiconducting behaviour.
The simulations have also been used to explore the evolutions of the structural and electronic properties in the liquid at very high pressures and temperatures. A progressive transition towards a metallic phase is observed which is linked to a less symmetric structure and a higher coordination number [4].
The similarities and differences of these features with those observed in the solid state will be discussed.
Finally, the effects of varying the composition x in $In_{1-x}Se_x$ alloys from semiconducting to metallic compositions were explored by AIMD-EXAFS [2]: the obtained concentration induced transition will be discussed in the light of the previous pressure/temperature induced one.

References

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