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High pressure XRD and XAS Study of SnI_4

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Thanks to nano-polycrystalline-diamond (NPD) anvils [1], high pressure X-ray absorption spectroscopy (XAS) at high energy is now accessible (no glitch in the spectra due to the single crystal diffraction of the anvils). Moreover, the high energy makes easier X-ray diffraction (XRD). In this presentation we will illustrate recent XAS results on SnI4, both at the Sn and I K edge combined with XRD. The EXAFS data have been fitted using the Reverse Monte Carlo (RMC) method implemented in the EVAX software.

SnI4 is a molecular crystal with Sn localized at the center of I4 tetrahedron. Under pressure it becomes metallic and amorphous. This was observed by XRD, resistivity measurements and Mössbauer spectroscopy [3]. Combining XRD and XAS on the same sample in the same pressure conditions, we have determined both the compressibility of the molecule and the compressibility of the lattice. From diffraction, an intermediate phase between the crystalline cubic ordered phase and the amorphous one has been observed. From the EXAFS data at the Sn K edge, a clear increase in the Sn-I distance is observed, already below 10 GPa. The situation for the iodine atom is more complicated. As second neighbors of iodine atom (Sn being the first), one can find two types of iodine: the first coming from the same tetrahedron (intra-connection) which means linked to the same Sn atom, the other one coming from the adjacent tetrahedra (inter-connection) which means linked to a different Sn atom. The RMC fit shows clearly that the inter-connection number increase with pressure and at 10 GPa the two type of Iodine neighbors are equally distributed. At this pressure XRD shows a broadened diffraction pattern, but still cubic. Above 15 GPa most of the Iodine participate to inter connections. At this stage, SnI4 is amorphous. Our results are roughly in agreement with the model proposed by Pasternak et al [3] (creation of chains of linked SnI4 tetrahedra) but with some differences in the transition pressures and in the final structure of the amorphous state.

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