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Amorphous–amorphous transition in SnI_4 reexamined

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The pressure-induced solid-state amorphization found in 1985 [1] set off a series of subsequent researches on polymorphism in SnI_4 . The discovery of another amorphous state [2], called Am-II to Am-I previously identified, on decompression became a breakthrough in solving the puzzle.

Later, a consistent thermodynamic argument has been given for the observed polymorphic behaviors [3]. However, the following questions remain unanswered: The ambient crystalline phase CP-I never transforms into Am-II, which appears only on Am-I decompression. Nonetheless, CP-I can directly transform to Am-I on recompression skipping CP-II [4], the high-pressure modification of CP-I.

We reexamined the Am-I-to-Am-II process conducting high-pressure synchrotron x-ray diffraction studies with a diamond anvil cell [5]. Detailed analysis of the structural evolution revealed that the association of molecules, which are entirely dissociated, starts at around 14 GPa on decompression. About 30% of isolated Sn atoms suddenly complete the molecular formation at the Am-I-to-Am-II transition at 3.3 GPa, associated with an abrupt drop of density. Thus, the molecules formed recover their original symmetry of T_d at the transition, implying the strong coupling between the global order parameter of density and the local symmetry.

Because the centers (Sn atoms) were distributed everywhere in Am-I, formed molecules' resulting location is not necessarily energetically optimized, leaving uniform distribution of shorter (2.64 Å) van der Waals I_2 bonds, which play as *defects*. The open questions are then understandable in terms of the defects. Crystallization of Am-II to CP-I could be a defect extinction process, but the reverse process would hardly occur. It seems impossible to remove the whole defects in recovering CP-I, and the residual defects prevent defective CP-I from reordering to CP-II, which may require highly ordered stacking of Sn layers [6].

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[6] H. Naruta *et al.*, J. Phys.: Condens. Matter **32**, 055401 (2019).

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