Polyamorphization induced superconductivity in Sb_2Se_3

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Pressure has been used as an effective tool to tune the structure and property of materials. The near room temperature superconductive was achieved recently at extremely high pressure with great help from the crystal structure prediction via first principles calculation. But the superconducting mechanism in disordered systems has been less in focus. Superconductivity and Anderson localization represent two extreme behaviors of electrons in condensed matter system. Surprisingly, these two competitive behaviors can occur in the same quantum system, e.g., amorphous superconductor. Although disorder-driven quantum phase transition has attracted much attention, the structure origins remain unclear. Here, by applying high pressure to amorphous Sb_2Se_3, we discover an unambiguous correlation between superconductivity and density up to 65 GPa. Superconductivity first emerges in high density amorphous (HDA) phase above 23 GPa when the glass density reaches crystalline Sb_2Se_3, and then becomes more prominent in the body-center-cubic (BCC) phase above 50 GPa. Upon decompression, superconductivity persists until a sharp density drop where BCC phase transforms back to low density amorphous (LDA). *Ab initio* simulations reveal that the BCC-like local geometry motifs form in HDA by increasing fractions of short atomic rings, which could simultaneously transform the covalent bonds into “metavalent bonds”, a recent classification of chemical bonding coined in chalcogenide materials. Our results demonstrate that the intermediate amorphous state is responsible for the incipient superconductor prior to normal superconductive behavior.

Keywords: superconductivity; amorphous density; metavalent