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INFLUENCE OF GE, PB, SB AND TE DOPANTS ON FERROELECTRICITY AND CRITICAL BEHAVIOR OF SN2P2S6 SEMICONDUCTOR CRYSTAL

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High resolution thermal diffusivity measurements have been carried out to precisely localize the ferroelectric to paraelectric phase transition of Sn2P2S6 crystal independently doped with Pb, Ge, Sb and Te at a low atomic percentage. Sn2P2S6 is a poor thermal conductor material, whose ferroelectricity comes from the stereochemical activity of the electron lone pair (5s2) of Sn cations, which is determined by hybridization with P2S6 molecular orbitals (3p4). Substitution of Sn by Ge makes this hybridization stronger improving the ferroelectricity, shifting the transition to higher temperatures and its shape becomes sharper. Introducing Pb instead of Sn affects in opposite manner, smearing the transition and lowering the critical temperature. This happens because there is a difference in the energy distance between Ge4s – S3p and Pb6s – S3p electronic levels. The influence of Sb was much smaller while that of Te was practically none because they, respectively, substitute non-ferroactive P and S ions in the crystalline network. The inverse of the thermal diffusivity has been used as a tool to study the influence of dopings (Ge, Pb, Sb and Te) on the evolution of the critical behavior in the vicinity of the second order phase transition. In all cases the ferroelectric phases are well described using the phenomenological Landau model based on a general mean-field approach. On the contrary, for the description of the paraelectric phase it was necessary to use a model which takes into account the first fluctuations correction to the Landau model and possible contribution of the charged defects, as it was previously found for Sn2P2S6. Moreover, the relative importance of the presence of charged defects increases significantly for Ge and Pb atoms. For Sb atoms the increase was less while for Te the value was practically the same as for pure Sn2P2S6.