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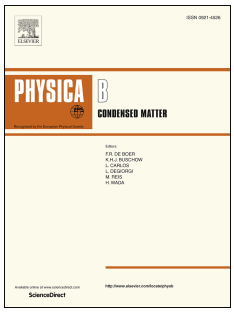

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Enhanced electrical transport properties via Pb vacancies in single crystalline PbTe prepared by Te-flux method

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Abstract

In PbTe system, Pb vacancies (V_{Pb}) are preferentially formed compared with other intrinsic point defects (anti-sites Te_{Pb} and interstitials Te_i) under the Te-rich condition. In order to explore the effect of V_{Pb} on electrical transport properties of PbTe thermoelectric material, the electronic structures of PbTe with V_{Pb} are determined by the first principle calculations. Theoretical calculations reveal that the V_{Pb} can modify the band structure near the Fermi level, which can increase the number of carrier pockets thus increase the carrier concentration. Based on the calculated results, single crystalline PbTe samples with V_{Pb} have been prepared by Te-flux method according to the stoichiometric ratio of $PbTe_{1+x}$ (x = 2.0, 2.5, 3.0 and 3.5). The experimental results show that carrier concentration is optimized significantly by tuning Te-flux content, and it varies from 2.94×10^{18} to 8.01×10^{18} cm^{-3}. The highest electrical conductivity reaches 3.1×10^{4} $S\cdot m^{-1}$ at 300 K for x = 3.5. A large Seebeck coefficient of 562 μV/K is obtained

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