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Dimensional crossover and thermoelectric properties in $CeTe_{2-x}Sb_x$ single crystals JONG-SOO RHYEE, Kyung Hee University, KYUNG EUN LEE, Samsungtechwin R&D Center, JAE NYEONG KIM, JI HOON SHIM, Pohang University of Science and Technology, BYEONG HUN MIN, YONG SEUNG KWON, Daegu Gyeongbuk Institute of Science and Technology — Several years before, we proposed that the charge density wave is a new pathway for high thermoelectric performance in In_4Se_{3-x} bulk crystalline materials. (Nature v.459, p. 965, 2009) Recently, from the increase of the chemical potential by halogen doped $In_4Se_{3-x}H_{0.03}$ (H=Halogen elements) crystals, we achieved high ZT (maximum ZT 1.53) over a wide temperature range. (Adv. Mater. v.23, p.2191, 2011) Here we demonstrate the low dimensionality increases power factor in $CeTe_{2-x}Sb_x$ single crystals. The band structures of $CeTe_2$ show the 2-dimensional (2D) Fermi surface nesting behavior as well as a 3-dimensional (3D) electron Fermi surface hindering the perfect charge density wave (CDW) gap opening. By hole doping with the substitution of Sb at the Te-site, the 3D-like Fermi surface disappears and the 2D perfect CDW gap opening enhances the power factor up to $x = 0.1$. With further hole doping, the Fermi surfaces become 3-dimensional structure with heavy hole bands. The enhancement of the power factor is observed near the dimensional crossover of CDW, at $x = 0.1$, where the CDW gap is maximized. This research was supported by Basic Science Research Program (2011-0021335), Mid-career Research Program (Strategy) (No. 2012R1A2A1A03005174) through the National Research Foundation of Korea (NRF) funded by the Ministry of Education, Science and Technology, and TJ Park Junior Faculty Fellowship funded by the POSCO TJ Park Foundation.

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