Nernst-Ettingshausen effect near zero energy gap in $Pb_{1-x}Sn_xSe$

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The Nernst- Ettingshausen (N-E) effect and electron mobility are investigated theoretically and experimentally in mixed $Pb_{1-x}Sn_xSe$ crystals as functions of temperature and chemical composition in the vicinity of vanishing energy gap E_g. The study is related to the discovery that, by changing the temperature, one arrives at the band ordering in which the topological crystalline insulator states appear on the surface [1]. It is shown theoretically and experimentally for four $Pb_{1-x}Sn_xSe$ samples having x between 0.25 and 0.39 that the bulk N-E effect reaches maximum value as a function of temperature when the energy gap goes through zero [2]. This result contradicts the claim made in the literature that, as the gap vanishes, the N-E effect changes sign [3].

The dc transport phenomena are successfully described theoretically in conditions of extreme bands' nonparabolicity. A situation is reached in which both 2D bands of topological surface states and 3D bands of the bulk crystal are linear in electron **k** vector. The theory uses a spherical approximation to the multi-ellipsoidal bands near the L points of the Brillouin zone. Pertinent scattering modes and their contribution to dc transport phenomena in $Pb_{1-x}Sn_xSe$ are analyzed to reach a proper description of our experimental transport results. Spin-flip scattering transitions for all modes are taken into account. As the gap goes through zero, some transport integrals exhibit a singular nonphysical behavior and it is demonstrated how to deal with this problem by introducing damping. Fitting the theoretical description to experiments in four samples we establish adjustable parameters for the active scattering modes. A very good agreement between the theory and experiment is obtained for critical temperatures at which the gap Eg vanishes for different chemical compositions.

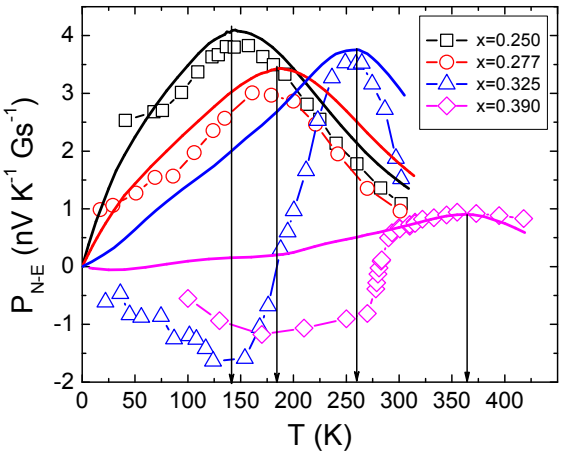

Figure 1: Theoretical and experimental P_{N-E} coefficients versus temperature for four investigated $Pb_{1-x}Sn_xSe$ samples. Solid lines - theory, open symbols - experiment. Vertical arrows point to the temperatures for which the corresponding gaps vanish.

[1] P. Dziawa et al, *Nature Materials* **11**, 1023 (2012).
[2] K. Dybko et al, *New J. Phys.* **18**, 013047 (2016).
[3] T. Liang et al, *Nature Commun.* **4**, 2696 (2013).