# Pressure-induced Lifshitz Transitions and superconductivity in doped topological insulator $Nb_xBi_2Se_3$

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Keywords: electronic topological transition, topological materials, superconductivity.

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The chemical doping or pressure-induced electronic topological transition (ETT) or Lifshitz transition is a change in the Fermi surface topology (FST) without symmetry breaking [1]. Unveiling of Lifshitz transition in solids is important for discovering new quantum matters, such as nontrivial semimetal [2,3], and the unconventional superconductivity [4-6]. The superconductivity is closely related to the Fermi surface change [7].

Recently, the doped topological insulators $M_xBi_2Se_3$ (M=Cu, Nb, Sr) are proposed to be potential topological superconductors [8], currently attracting more interest. However, whether the pressure-induced ETT exists in $Bi_2Se_3$-based topological materials or not is still uncertain. Among them, the Nb-doped $Bi_2Se_3$ is distinct from the others, especially for the multiple Fermi surfaces originating from the hybridization between partially occupied Nb-4$d$ states and the Bi/Se-$p$ orbital states near Fermi level [9,10]. From a band theory perspective, the $Nb_xBi_2Se_3$ material is a heavily doped narrow-gap semiconductor, whose electronic states are expected to be highly susceptible to external pressure. Given the unique multiband structures and layered crystal structure in Nb-doped $Bi_2Se_3$, it provides an tunable platform for accessing the Lifshitz transition in $Bi_2Se_3$-based topological materials.

In this work, we elucidated a rare example of multiple Lifshitz transitions relevant to three distinct energy bands below 12.0 GPa in the rhombohedral phase of $Nb_xBi_2Se_3$ using a combination of electrical transport, synchrotron x-ray diffraction, Raman scattering spectroscopy measurements and first principle calculations. We show the emerging multibands at the Fermi level from hybridizing the Nb-4$d$ and Bi/Se-$p$ orbital states are critical for our findings. The phase diagram was obtained as shown in Figure 1 (a)-(b). Two first-order structural phase transitions of rhombohedral-monoclinic and monoclinic-tetragonal phase were assigned just above 12.0 GPa and 22.3 GPa, respectively. Contrast to filamentary superconducting state below 22.9 GPa, we demonstrated zero resistance superconductivity and a semi-dome shape pressure dependence of transition temperature $T_c(P)$ in tetragonal phase. Furthermore, we demonstrate the first evidence of multiband superconductivity in pressurized $Nb_{0.25}Bi_2Se_3$, which may be ascribed to multiple Fermi surfaces associated with Nb-4 $d$ orbital states. Our results suggest the external pressure can provide an alternative effective strategy for tuning desired electronic states in doped topological insulators beyond further chemical doping and electric-field gate technique.

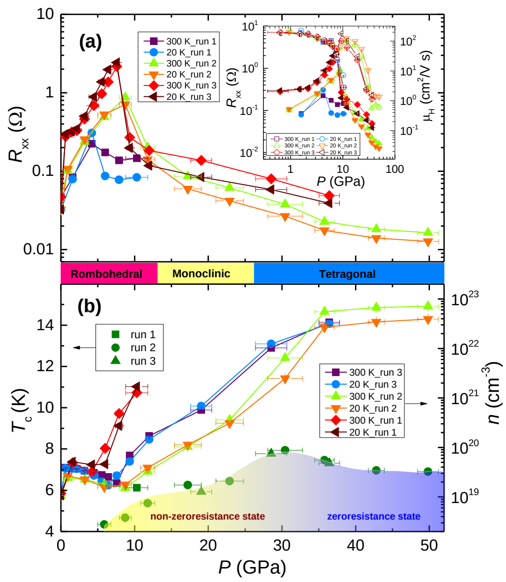


*Figure 1*. Phase diagram (a) $R_{xx}(P)$ at 20 K and 300 K. (b) $T_c(P)$ and $n(P)$ for runs 1-3. The inset of (a) shows the corresponding log-log plot including $\mu_H(P)$.

**Acknowledgments**: This work was supported by NSFC (grant No. 11804011).

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