

Supporting Information

Synthesis and thermoelectric properties of defected PbSe-PbTe heterojunction nano-structures

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Theory of Geometric phase analysis

Geometric phase analysis (GPA) was first published in Ultramicroscopy by M. J. Hytch^[1]. GPA was based on high-resolution transmission electron microscopy (HRTEM) image. An HRTEM image formed at a zone axis of a crystal can be considered as a set of interference fringes corresponding to the atomic planes of the specimen. GPA analyses these interference fringes individually to extract the information concerning strain. The method is based on the calculation the local Fourier components of lattice fringes. The phase of these local Fourier components, or geometric phase $P_g(\mathbf{r})$ is directly related to the components of the displacement field, $\mathbf{u}(\mathbf{r})$, in the direction of the reciprocal lattice vector, \mathbf{g} :

$$P_g(\mathbf{r}) = -2\pi\mathbf{g}\cdot\mathbf{u}(\mathbf{r})$$

Preparation of PbSe-PbTe HNPs with PEDOT:PSS

Firstly, 0.1 g PbSe-PbTe HNPs was adding into 10 g ethanol, and then it was sonicated for 30 minutes at room temperature. Secondly, an appropriate amount of DMSO was mixed with the PEDOT/PSS solution to form 5 wt % of DMSO/ PEDOT:PSS mixture. 5 g of PbSe-PbTe HNPs (dispersed in ethanol) and 5 g the above mixture (5 wt % of DMSO/ PEDOT:PSS) was mixed and sonicated for 30 minutes to form the mixture. A piece of cotton (2 cm × 2 cm) was dropped into the mixture and sonicated for 30 minutes. Finally, the cotton being treated was dried for 15 minutes at 130 °C. The sample been characterized was prepared.

Ref [1]: M.J. Hytch, E. Snoeck and R. Kilaas. Quantitative measurement of displacement and strain fields from HRTEM micrographs, *Ultramicroscopy*, **1998**, 74, 131-146.

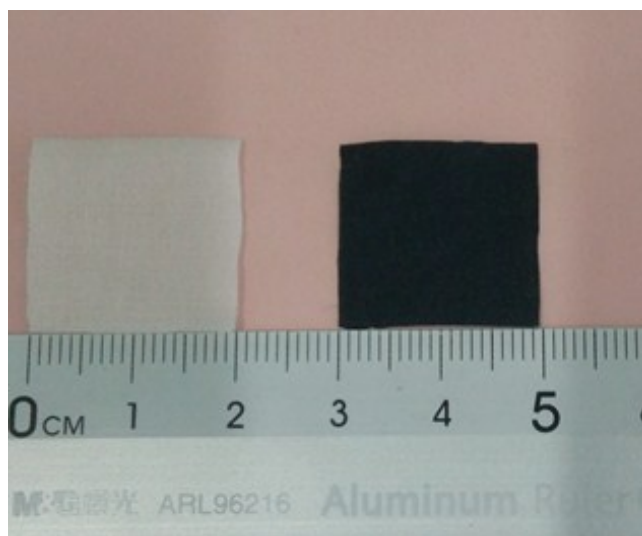


Fig. S1 Photograph of square cottons without and with PbSe/PbTe mixing poly(3,4-ethylenedioxythiophene) PEDOT : poly(styrenesulfonate) (PSS).

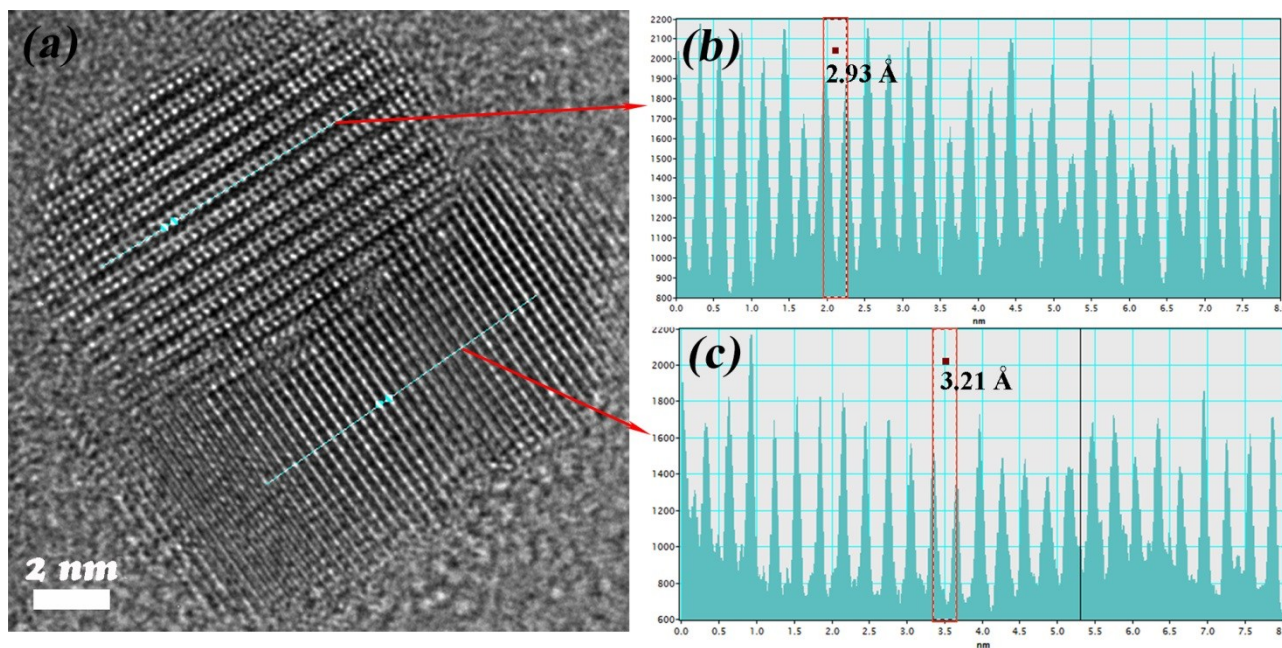


Fig. S2 (a) High-resolution TEM image of defected PbSe/PbTe heterojunction nanostructure. (b) and (c) are the interplanar spacing of PbSe and PbTe, respectively.

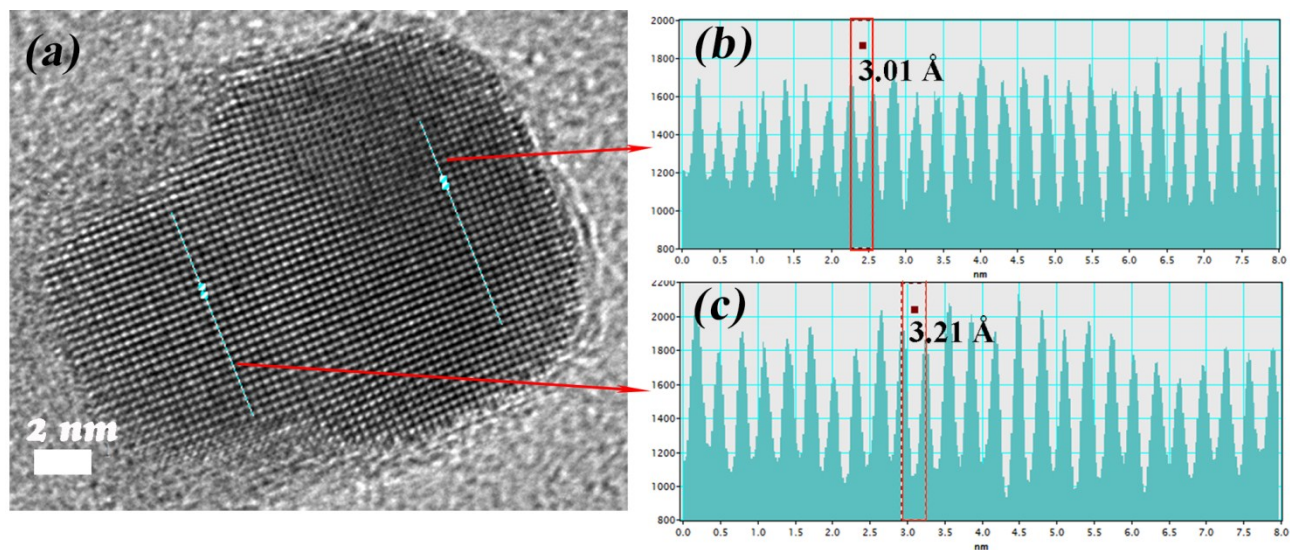


Fig. S3 (a) High-resolution TEM image of defect-free PbSe/PbTe heterojunction nanostructure. (b) and (c) are the interplanar spacing of PbSe and PbTe, respectively.

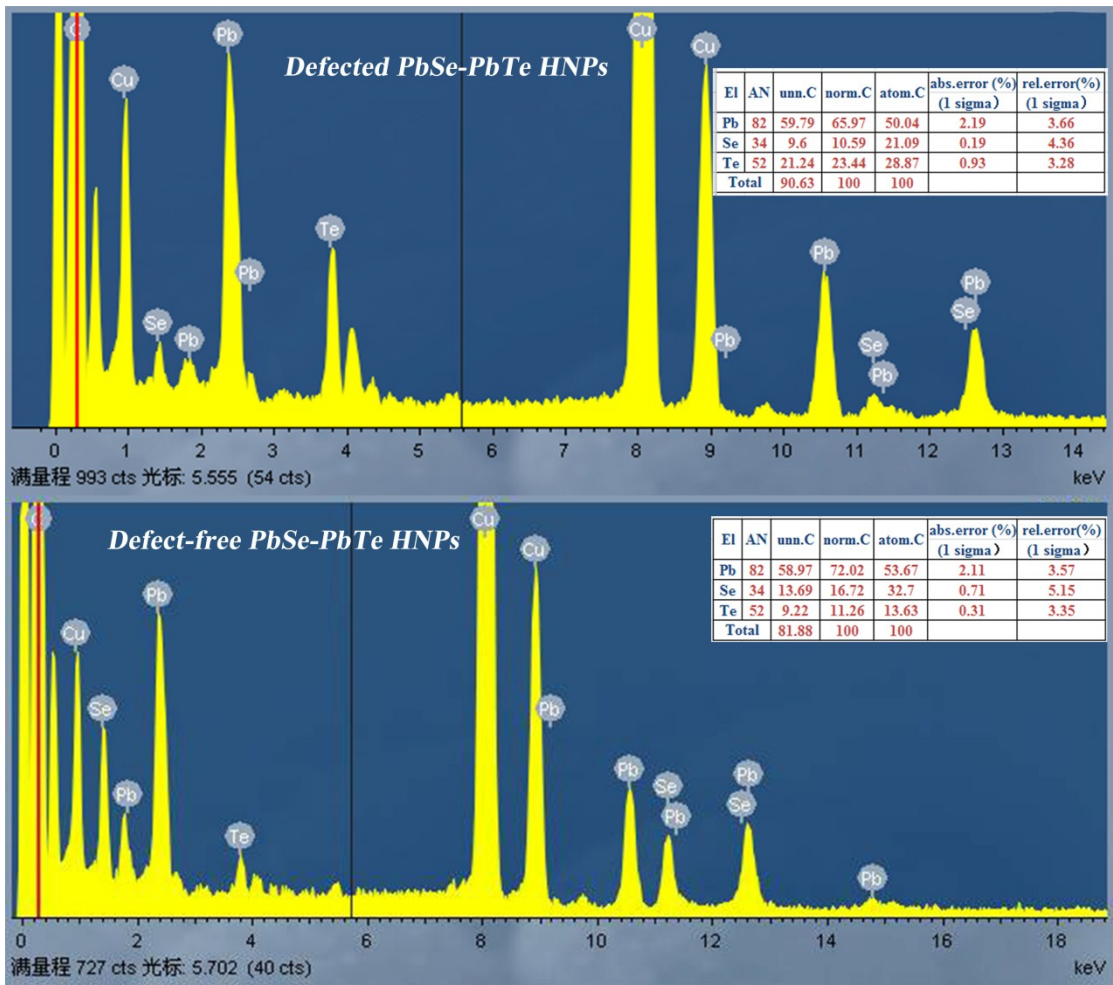


Fig. S4 EDS pattern and data of the defected and defect-free PbSe-PbTe HNPs.

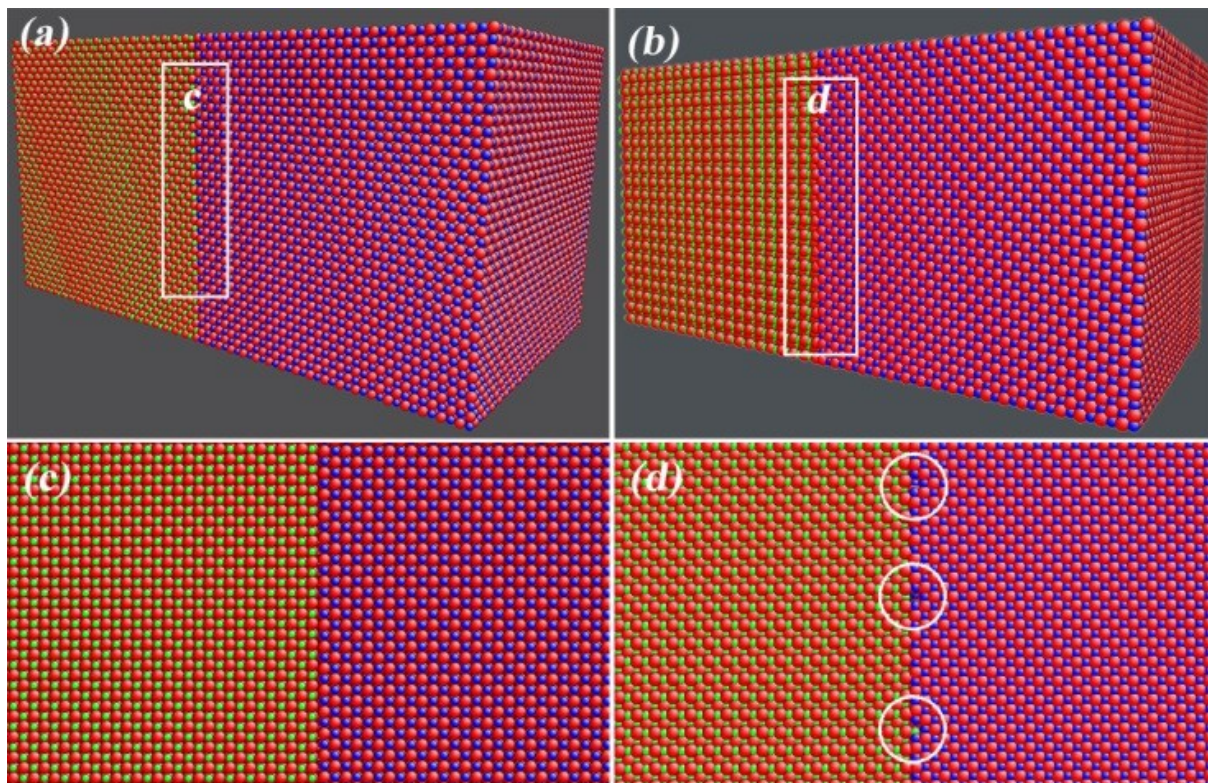


Fig. S5 The possible atomic model corresponding to the defected and defect-free PbSe-PbTe HNPs. (a) and (b) the 3D atomic model structures; (c) and (d) the 2D plane and the interface atomic model structures.