Electronic Supplementary Information

Phonon Dispersion and Electronic Structure In Quasi-one-Dimensional Layered Ta_2NiSe_7 Single Crystal

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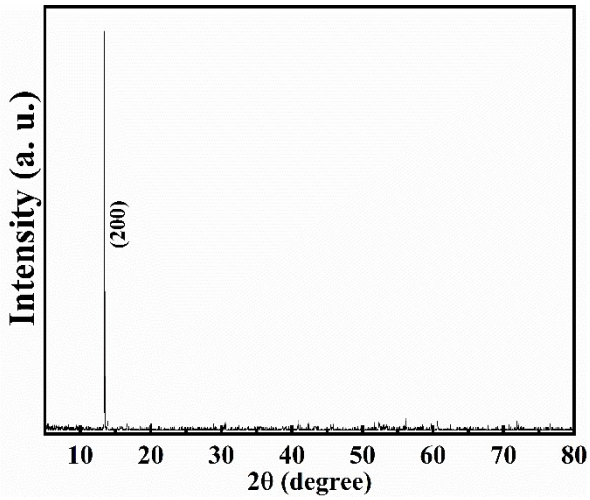

Fig. 1 The X-ray diffraction pattern of single crystal Ta_2NiSe_7, which was obtained from the naturally exposed crystal face.

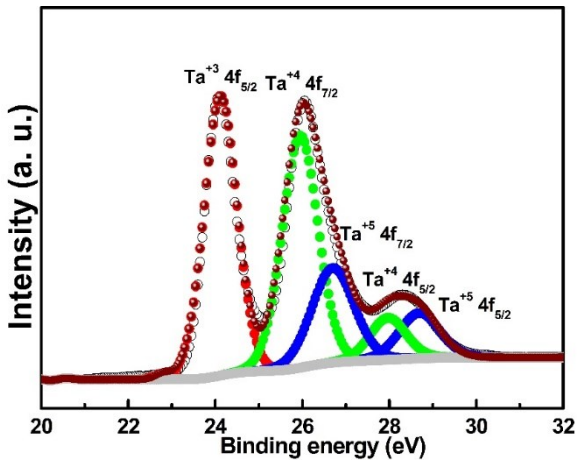

Fig. 2 XPS for the valence states of 4f states of Ta element

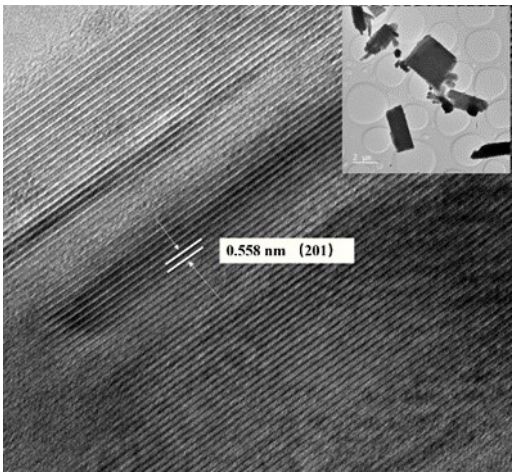

Fig. 3 TEM image of single crystal Ta_2NiSe_7, the corresponding interplanar spacing and diffraction index were also given

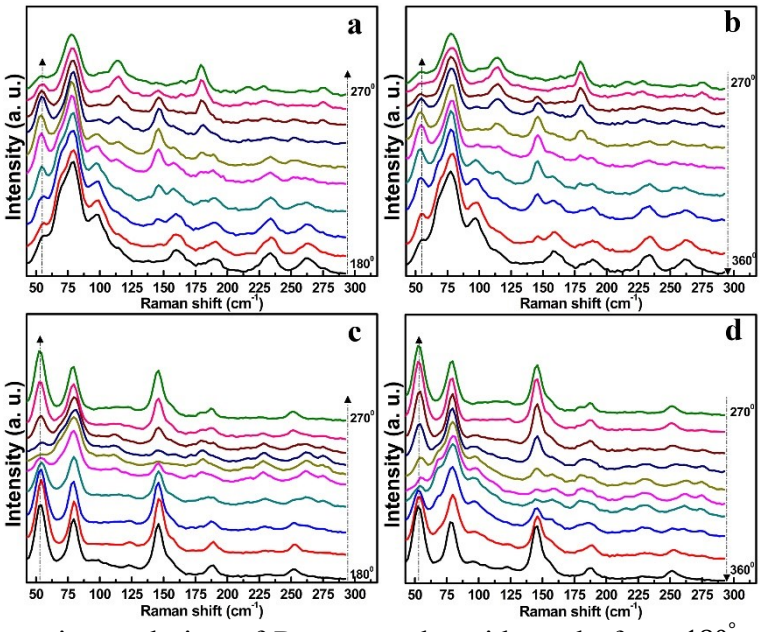

Fig. 4 The intensity evolution of Raman peaks with angle from 180° to 360° for the (100) crystal plane, (a-b) parallel polarization, (c-d) vertical polarization.

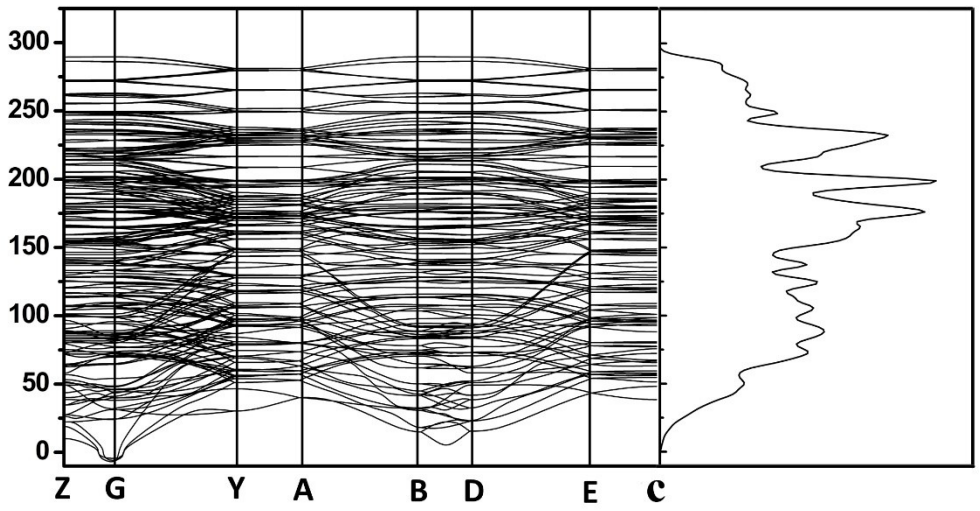

Fig. 5 Phonon dispersion spectrum and corresponding density of state (DOS) for layered Ta_2NiSe_7.

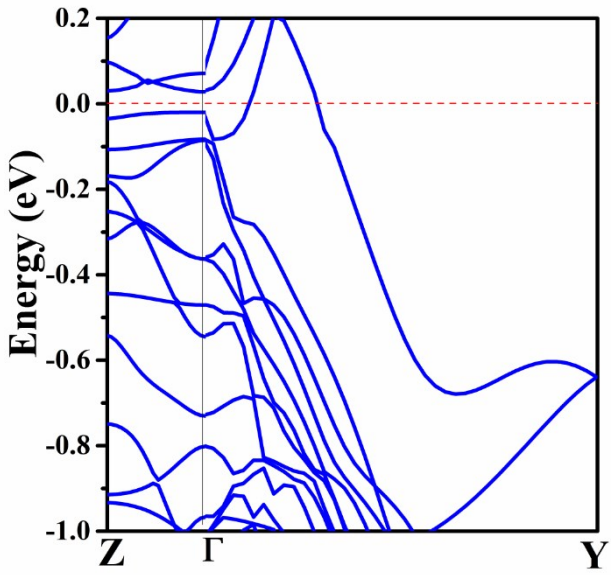

Fig. 6 The band structure of layered Ta_2NiSe_7 calculated by density functional theory using HSE06 functional

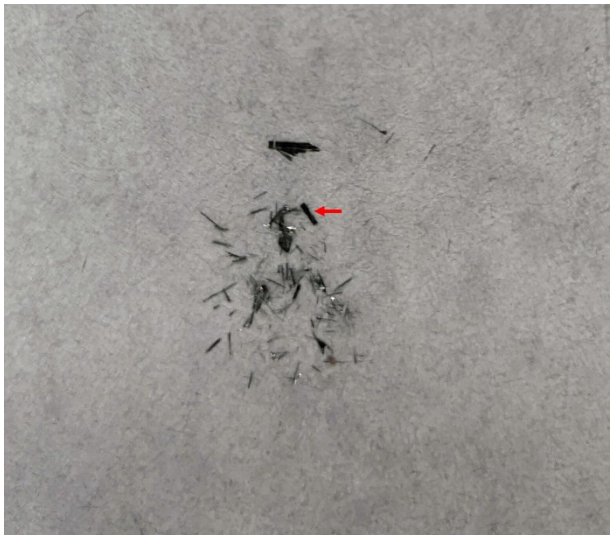

Fig. 7 The synthesised Ta_2NiSe_7 single crystal sample with about 2mm×8mm size.