

**Supplementary Material to the article**  
**“Interaction of charge density waves in the monoclinic phase of NbS<sub>3</sub>”**

**About twinning in NbS<sub>3</sub>-II.**

The choice of a twinning element based on a diffraction pattern is always ambiguous. At least because the diffraction pattern has a center of symmetry and does not allow one to distinguish a reflection in a plane from a 180-degree rotation around a perpendicular axis. In the article we comment Fig 1a in terms of the lattice. For an unambiguous choice one should switch from a lattice to a crystal structure consideration.

The NbS<sub>3</sub>-II structure is layered, with covalent bonds between atoms within the layers. Layers parallel to the *bc* planes are bonded by van der Waals forces. Such layered structure is typical of chalcogenides, in particular, of TiS<sub>3</sub>, which is a structural analogue of NbS<sub>3</sub>-I and is studied in detail. It is shown [1] that twinning in TiS<sub>3</sub> occurs along a plane parallel to the layers and is repeated many times, sometimes every few layers, which makes the TiS<sub>3</sub> structure highly defective. We believe that NbS<sub>3</sub>-II twins in a similar way. This is the main reason why the diffraction patterns are rather noisy.

### Distribution of main and satellite reflections in sections of the diffraction pattern.

Below we place extra X-ray diffraction data, which can give a more extensive picture of the structure and superstructures.

The following sections with  $k=\text{const}$  complement the section presented in Fig. 1a from the main text ( $k = 0$ ).

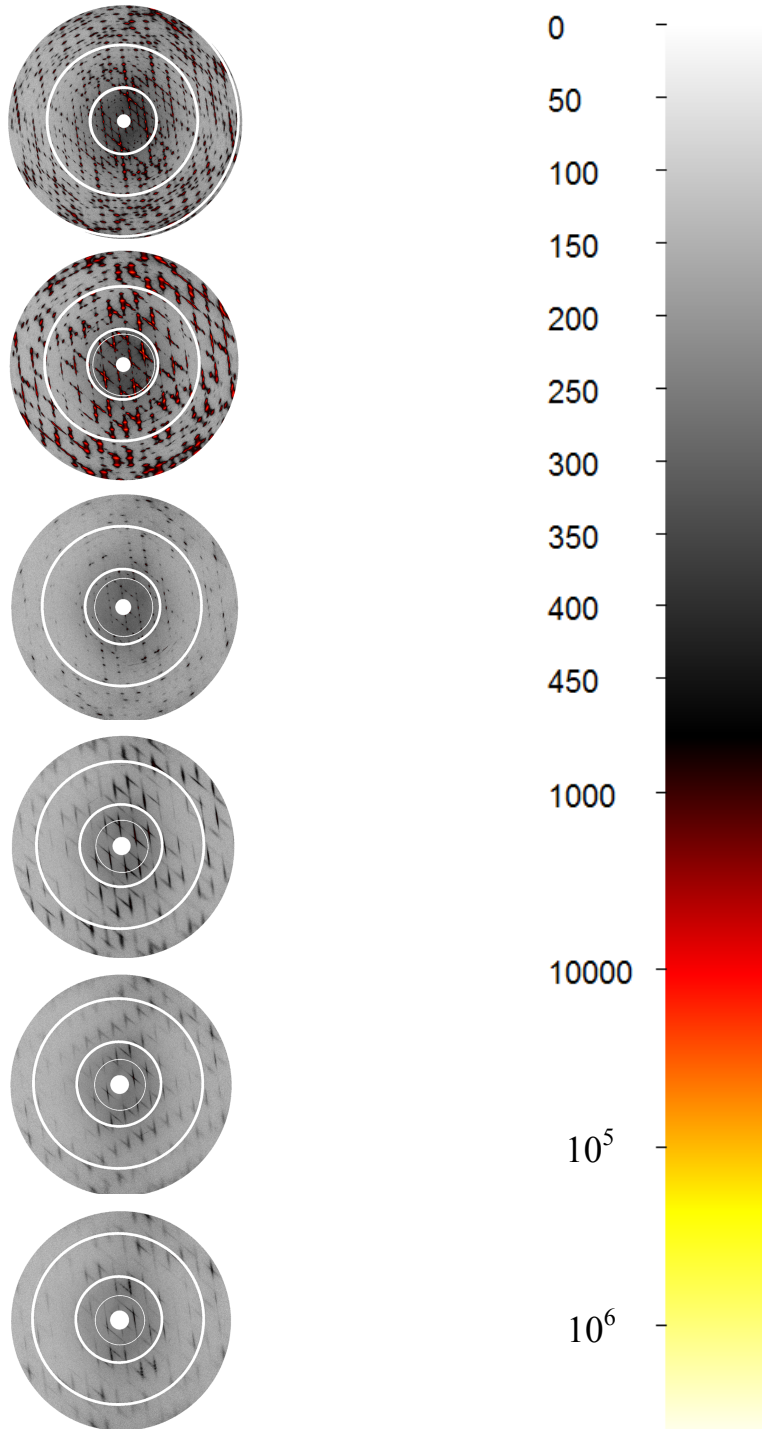


Fig. S1. Sections of the diffraction pattern of NbS<sub>3</sub>-II by planes  $k = \text{const}$ . From top to bottom:  $k= 1.30, 1.35, 1.40, 1.48, 1.50, 1.52$ .  $T=200$  K

The following sections complement the diagonal section  $(-h k h)$  presented in Fig. 1b from the main text. These figures, as well as Fig. 1b, show satellite reflections with fractional  $k$ -indices at several levels along the  $\mathbf{b}^*$  axis.

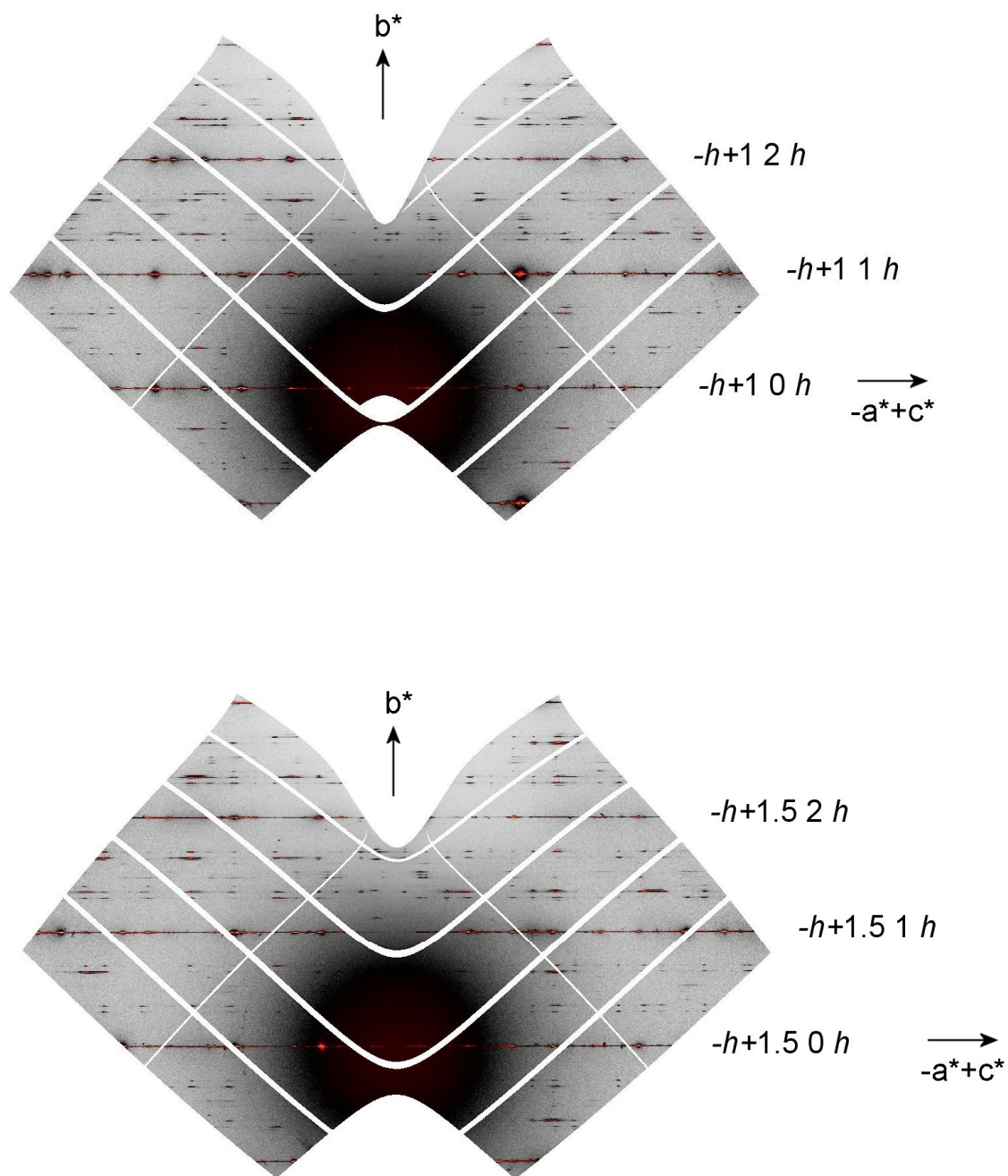


Fig. S2. Sections of the diffraction pattern of  $\text{NbS}_3\text{-II}$  by planes  $(-h+1 k h)$  (top) and  $(-h+1.5 k h)$  (bottom).  $T=200$  K

### The temperature map for the second harmonic of $\mathbf{q}_1$ .

Here we present the temperature map of reflections with  $k = 0.4$ . They disappear above 270 K. At this temperature a transition occurs, whose nature remains to be determined. Interestingly, at the same temperature the second harmonic of  $\mathbf{q}_0$  also weakens sharply (Fig. 2 (c) from the main text).

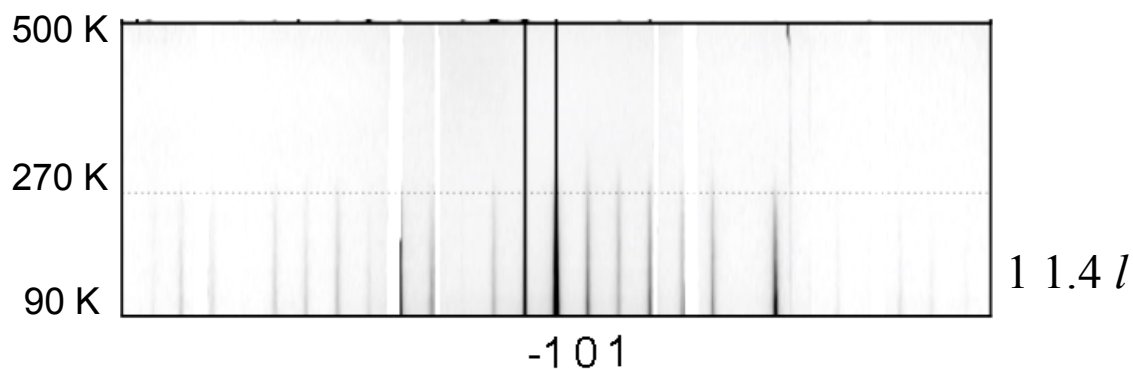


Fig. S3. Temperature dependences of the intensity of satellite reflections in the range  $T= 90\text{--}500$  K, plotted along the line  $1\ 1.40\ l$ . The indices correspond to the vector  $\mathbf{1-2q}_1=(0\ 0.4\ 0)$ .

1. I.N. Trunkin, I. G. Gorlova, N. B. Bolotina, V. I. Bondarenko, Y. M. Chesnokov and A. L. Vasiliev, *J. Materials Science*. **56**, 2150 (2021). doi: 10.1007/s10853-020-05357-0