Local analysis of periodically modulated structures

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While many low-dimensional systems exhibit charge density wave modulations, sliding of charge density waves (CDWs) has been proven only in a few components, including $NbSe_3$ and NbS_3-II. They form crystals in which quasi-one-dimensional chains are connected in layers separated by van der Waals gaps. Because NbS_3-II grows in the form of thin, needle-like crystals, its basic and CDW modulated structures were only recently determined [1] using a combination of several techniques.

Both materials are also each modulated by two wave vectors with only slightly different components along the chains. While diffraction techniques clearly show that both CDWs are present at sufficiently low temperatures, it is impossible to rule out the possibility of nanometer-sized domains with different modulations without real space information. We revisit this topic using low temperature Scanning Tunneling Microscopy (STM) on $NbSe_3$ samples cleaved in UHV. Performing 1D Fourier transform analysis along the crystal chains on long enough images with atomic resolution guarantees the necessary k-space resolution in combination with real space information, making it possible to unambiguously determine the presence of CDW modes on individual columns [2]. In addition, this allows for quantitative comparison of modulation amplitudes on different chains of the same type at different scanning parameters and studies of modulation variations along individual columns.

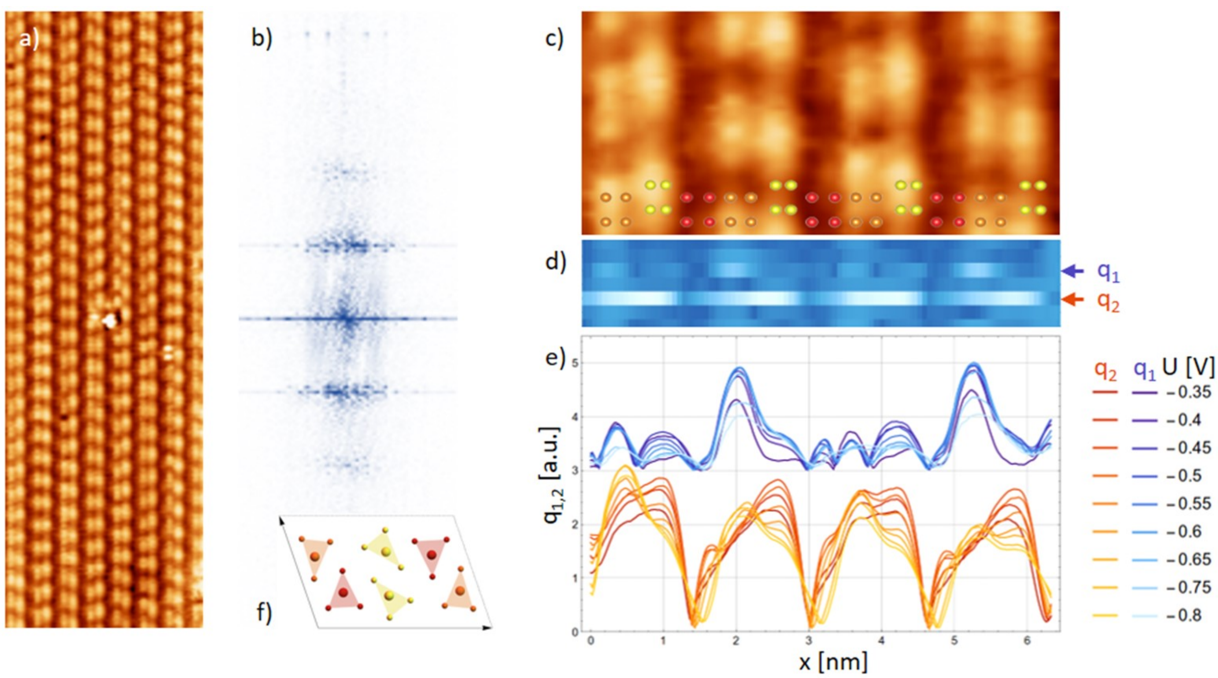

Figure 1. a) STM image of the surface of $NbSe_3$, together with its 2D Fourier transform in b). The surface structure is overlaid on a part of the STM image c). d) Results of 1D Fourier transform along the chains (parallel to $\mathbf{b_0}$) clearly show the presence of both modulation wave-vectors q_1 (blue) and q_2 (red). Their intensity profiles are ploted in e).

[1] E. Zupanič et al., PRB **98**, 174113 (2018).

[2] M. A. van Midden et al, PRB **102**, 075442 (2020).

Keywords: Charge density waves, Low-dimensional structures, $NbSe_3$, NbS_3-II, Scanning Tunneling Microscopy

The authors would like to thank S. Šturm, E. Tchernychova, V. Ya. Pokrovskii, S. G. Zybtsev, V. F. Nasretdinova, S. V. Zaitsev-Zotov, W. T. Chen and Woei Wu Pai, J. for their invaluable contributions.