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Crystallographic Aspects of the CDW Instabilities in NbSe₃

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Charge-density waves (CDW) in some quasi one-dimensional compounds can be depinned from the lattice by an external electric field. In the case of NbSe₃, two CDW transitions have been reported with onset temperatures of 144 K and 59 K. From an analysis of the published low-temperature (LT) scanning tunneling microscopy (STM) images, which inherently allow the resolution of domain structures on the atomic scale, an alternative model of the CDW modulated structures in NbSe₃ is proposed. In contrast to the existing model, where two incommensurate (IC) modes, $q_1 = (0, 0.241, 0)$ and $q_2 = (0.5, 0.260, 0.5)$ are selectively confined to two of three available structurally distinguished types of bi-capped trigonal prismatic columns, the alternative model [1,2] proceeds from the assumption that both columns of the same pair are alternatively modulated by the two modes, whose IC components add within experimental error into a commensurate value. The observed domains are formed as a result of the different bonding within and between the structural layers, separated by Van der Waals gaps, and of the ability of the two modes to be easily interchanged between two symmetry-related columns of the same type. This assumption is in accord with the published LT STM results, which confirm i.a. the presence of both IC modes above 59 K, where according to the previous model only the q_1 contribution should be expected. A pair of two alternatively modulated columns of the same type represents the basic structural unit of the CDW ground state. The two modes can formally be replaced by a single inharmonic modulation, obtained by “beating” between the two IC modes.

[1] Prodan A., Midden van H. J. P., Žitko R., Zupanič E., Bennett J.C., Böhm H., *Sol. State Comm.* (2010). 150, 2134., [2] Prodan A., Midden van H. J. P., Zupanič E., Žitko R., *Mater. Sci. and Eng. Forum, Solid State Phenomena* (2013). 203-204, 42.

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