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The CDW modulated structure of NbSe3

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NbSe3 undergoes two charge-density wave (CDW) transitions with incommensurate (IC) modes q1 = (0,0.241,0) (at T1=144K) and q2 = (0.5,0.260,0.5) (at T2=59K). There is sufficient experimental evidence [1,2] that the two modes appear pair-wise along one (at T1) or along two (at T2) symmetry-related pairs of trigonal prismatic (TP) columns, which form together with the third, unmodulated pair, the basic structure of the compound. The apparent sliding of the two modes in the presence of an electric field is a result of an easy switching between the two modes and consequently of the dynamics of the unstable layered domains. The relatively rare property of CDW sliding is thus a direct consequence of the specific basic structure of NbSe3 and the related compounds. Since the thickness of these domains is extremely small, of the order of the Se-Nb-Se sandwiches, any structural information, obtained by classical diffraction methods, should be confirmed by an alternative method, such as scanning tunneling microscopy (STM), having both resolution and sensitivity on an atomic scale.
This new explanation of the modulated ground state of NbSe3 appears to be in good accord with a series of experiments performed on this compound. In addition, ab-initio (DFT/VASP) calculations are under way to confirm the model. The two IC modes can formally be replaced by a single, highly anharmonic modulation, obtained by "beating"between the two, which replaces both individual modes along all modulated columns.

References
[1] A. Prodan et al., Sol. State Comm. 150, 2134 (2010).
[2] A. Prodan et al., Mater. Sci. and Eng. Forum, Solid State Phenomena, Appl. Cryst. XXII, 203-204, 42-47 (2013).

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