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Superlattice Formation and Charge Density Waves in $\text{TiSe}_{2-x}\text{Te}_x$

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— Charge density waves (CDW) are spatial modulations of electron density that are accompanied by a periodic lattice distortion that creates a superlattice. Many layered structures such as transition metal dichalcogenides undergo temperature dependent CDW transitions. TiSe_2 has a much studied but still not completely understood transition below 200K. The origin of charge density waves (CDW) in TiSe_2 is controversial, with exciton formation and an indirect Jahn Teller effect as leading candidates to be the driving force behind the transition. Neutron scattering experiments were carried out at NOMAD at Oak Ridge National Lab and BT-1 at NIST Center for Neutron Research to investigate the effect of tellurium doping on the CDW transition in $\text{TiSe}_{2-x}\text{Te}_x$. Finding the composition dependence of the transition is instrumental in understanding what drives the phase change. Using pair distribution function analysis of the local structure, peak splitting shows that the nominal hexagonal unit cell is insufficient to describe the high temperature phase and a monoclinic cell must be used. Rietveld refinement of BT-1 data shows that phase change continues to occur with increased concentrations of Te.

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