Effects of electron-beam generated lattice defects on the structure of charge density waves in 1T-$TaSe_2$, and 1T-TaS_2

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Charge density waves (CDW) are periodic modulations of charge density in low-dimensional metals as a function of temperature, doping and pressure. CDWs are coupled to a periodic lattice distortion (PLD) which is the periodic modulation of atomic positions.[1] CDW can be directly probed using Scanning Tunnelling Microscopy (STM). On the other hand, imaging and diffraction techniques such as High Resolution Transmission electron Microscopy (HRTEM)x-ray and electron diffraction are sensitive to the PLD.[1] Theory has shown that an incommensurate CDW should exhibit frictionless sliding in an electric field, leading to Froehlich type superconductivity.[2] However, Froehlich superconductivity is rarely observed since the sliding CDW is often pinned by crystalline impurities and defects.[2, 3] To understand transport properties in CDW materials it is crucial to investigate the interaction of the CDW with crystalline defects and impurities.

Here we report on the interaction of commensurate CDW/PLD with lattice defects generated by the electron beam in 1T-$TaSe_2$ and 1T-TaS_2.[4] Bulk 1T-TaS_2 and 1T-$TaSe_2$ are characterized by a commensurate CDW at 180 K and 300 K respectively. This gives rise to a $(13)^{0.5}$ x $(13)^{0.5}$ super lattice Figure 1(a) displays a HRTEM image of 1T-$TaSe_2$ obtained at 100 K. A Fast Fourier Transform (FFT) of the HRTEM image shown in fig 1(b) has spots from the main structure (solid red circles) surrounded by six satellite spots (dotted circle) from the PLD. Masking the satellite spots from the PLD, followed by inverse FFT helps to visualize the structure of the $(13)^{0.5}$ x $(13)^{0.5}$ superlattice arising from the commensurate PLD. The image showing the PLD maxima is presented in fig 1(c).

Figures 1(d)-(f) show successive HRTEM images obtained over time. The corresponding PLD images are shown in figures (g), (h), (i) respectively. It can be seen that the PLD becomes more disordered with increased exposure to the electron beam. A radial distribution function (RDF) showing the nearest-neighbor and next-nearest-neighbor periodicities between the PLD maxima was also calculated. The RDF in figures (j), (k), (l) have been calculated from the PLD images in figs. (g), (h), (i) respectively. The peak with the asterix shows the main periodicity due to the CDW/PLD wave-vector $|\mathbf{q}_{i=1"6}| = (13)^{0.5}\, a_0$ where a_0= lattice parameter =3.447 Å. Increased loss of long-range order with increased exposure to the electron beam leads to broadening of RDF peaks in regions marked with dotted rectangle in fig. 1(k) and fig.1 (l). We discuss the interaction of the CDW with the Friedel oscillations arising from the lattice defects caused by the electron beam. [2, 4]

References:

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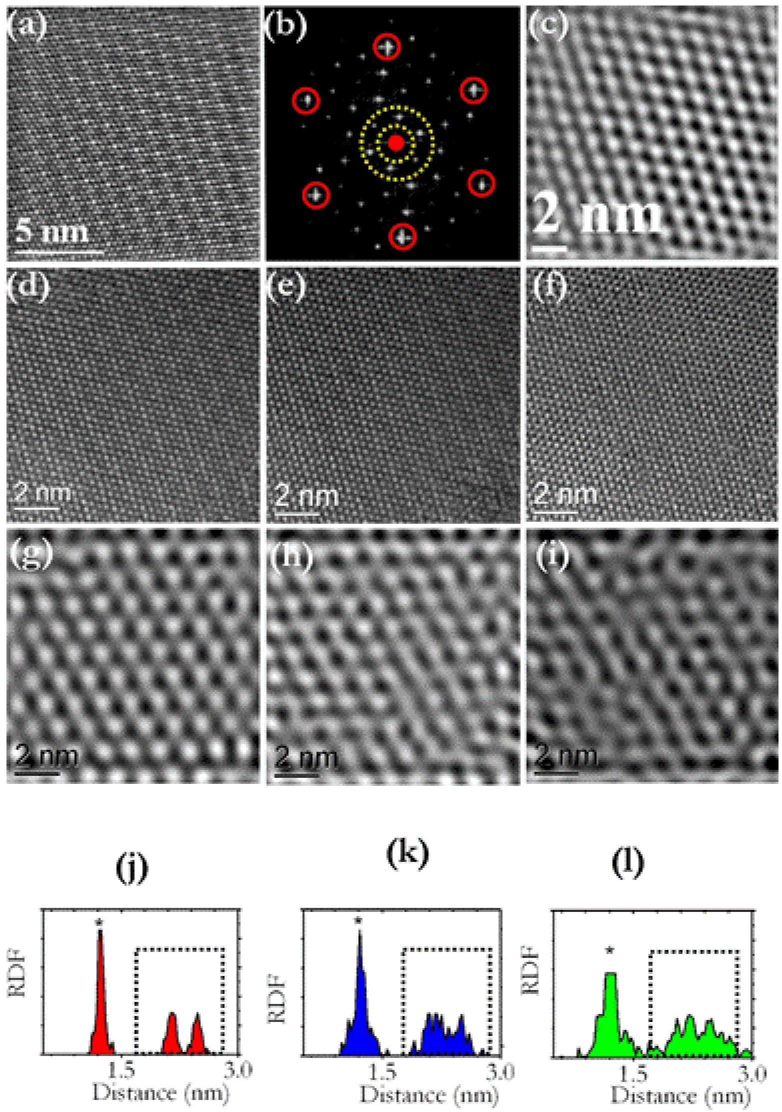

FIG. 1. (a) HRTEM image of 1T-$TaSe_2$ at 100 K (b) Fast Fourier Transform (FFT) of the HRTEM image showing the spots from the 1T-$TaSe_2$ structure (solid red circles) surrounded by six satellite spots due to the commensurate PLD (dotted circle). (c) The PLD maxima obtained from the HRTEM image showing a $(13)^{0.5}$ x $(13)^{0.5}$ superlattice. (d)-(f) Successive HRTEM images taken over time (g)-(i) Corresponding PLD lattices. (j)-(l) Radial distribution function (RDF) calculated from the PLD images showing the evolution of nearest-neighbor and next-nearest neighbor periodicities with increased exposure. The peak with the asterix shows the main periodicity due to the CDW/PLD wave-vector $|\mathbf{q}_{i=1"6}| = (13)^{0.5}\, a_0$ where a_0 is the lattice parameter for 1T-$TaSe_2$