Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Vacancy-induced growth of inversion domains in transition-metal dichalcogenide monolayer: an atomic view of defect dynamics JUNHAO LIN, Vanderbilt University/ORNL, WU ZHOU, ORNL, SOKRATES PANTELIDES, Vanderbilt University — In this work, we systematically study the nucleation and growth of inversion domains within a monolayer $MoSe_2$. We use a focused electron beam to generate and excite Se vacancies in the monolayer, and monitor their dynamics through sequential atomic-scale Z-contrast imaging. We find that Se vacancies are first randomly created and then preferentially agglomerate into line defects under the energy transferred from the electron beam. Successive evolution of these line defects induces nucleation of distinct triangular inversion domains within the $MoSe_2$ layer and generates conductive 60° grain boundaries within the semiconducting matrix. Density functional theory shows that the nucleation of inversion domain lowers the system energy due to the release of vacancy-induced lattice shrinkage. Migration of the grain boundaries can be further activated by deformation of the peripheral lattice, giving rise to the growth of the inversion domain. The grain nucleation and growth process observed under energy transferred from the electron beam can provide new insights into the structural stability of TMDC monolayers under severe (e.g. high temperature) working conditions.

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Date submitted: 13 Nov 2014 Electronic form version 1.4