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Atomic Scale Insights Into Dynamic Phase Changes in 2D Materials During In-Situ Thermal Processing

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2D materials comprised of more than one element are usually only one of many stable phases, and adopt the layered van der Waals structure. Many of the other stable phases present in the phase diagrams of two elements are not layered systems and form 3D bulk crystals. Growing ultrathin films of non-layered materials is very difficult as they prefer to adopt 3D geometry rather than 2D forms. However, by manipulation of the elemental stoichiometry it should be possible to drive phase changes from layered to non-layered systems.

Transition metal dichalcogenides (TMDs) 2D layered materials combine two elements, one metal and one chalcogen, and the chalcogen can be selectively removed from the material by heating. Heating releases chalcogen atoms first, leaving behind the heavier metal atoms. This mechanism of heating induced preferential chalcogen depletion opens up new opportunities to explore phase changes in few layered 2D TMDs and studies to reveal the atomic mechanisms and new phases produced. Since the starting 2D materials that are mono or few layer are already very thin (<5nm), the phase change to non-layered systems is likely to yield ultrathin forms of materials that cannot be easily produced using bottom up growth methods directly.

To explore this concept, an in-situ heating holder is used inside the Transmission Electron Microscope (TEM), with the ability to study temperatures up to 1200^{o}C, and obtain dynamic atomic scale images of the structures. The starting material explored is the Noble Metal Dichalcogenides, with Pd and Pt as the metals and Se and S as the chalcogens. The results show that new monolayer phases of Pd_2Se_3 are formed by heating $PdSe_2$ inside the TEM, and that unique 1D void channels are produced [1]. The striated lattice in Pd_2Se_3 exhibits thermal processing differences to commonly studied TMDs of MoS_2 and WS_2 which tend to simply form defect clusters and at some point metal nanoparticle clusters. Pd-Se has a rich phase diagram with many stable phases with exotic lattice structures that enables the fabrication of novel nanoscale structures using PdSe2 as the starting template. Comparisons will be made with $PtSe_2$ and $ReSe_2$ to show how different layered systems undergo thermally driven phase transformations when chalcogen is depleted. Grain boundaries and fundamental defect structures of the new ultrathin materials will be presented. Finally, it will be shown that similar thermally driven effects can be achieved in $PdSe_2$ using focused laser irradiation [2].

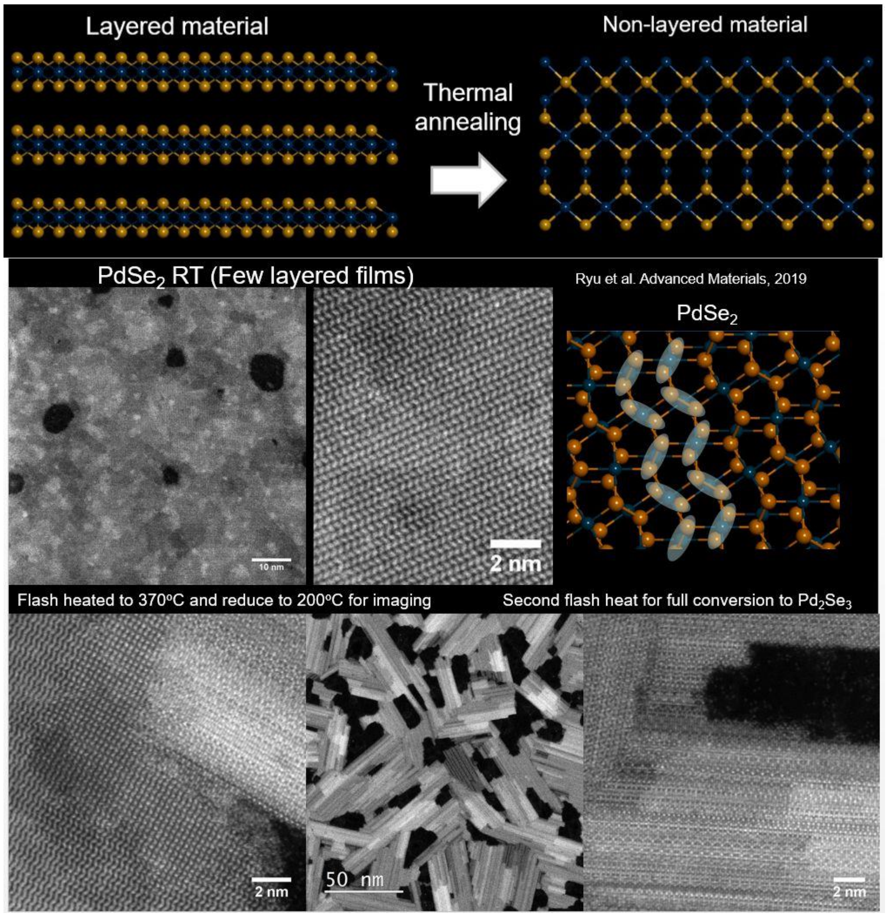

Figure 1. Phase transformation of $PdSe_2$ using in-situ heating in TEM

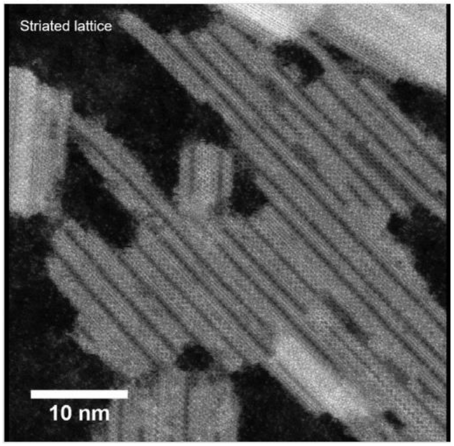

Figure 2. Striated lattice voids in Pd_2Se_3 after $PdSe_2$ phase transformation induced by heating.

References:

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