Atomic Structure, Stacking, and Stability of Two-Dimensional Gallium Selenide Telluride Crystals

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Abstract

Two-dimensional (2D) layered III-VI materials (i.e. GaSe, GaTe) are bright light emitters in a variety of thicknesses, contrary to most studied transition metal dichalcogenides (i.e. MoS₂, WS₂) that are efficient light emitters only in single layer form^[1]. Bulk Gallium Selenide (GaSe) has a hexagonal structure with an indirect bandgap of 2.0-2.1 eV, while bulk Gallium Telluride (GaTe) has a monoclinic structure with a direct band gap of 1.7 eV^{[1][2][3]}. When thinned down to mono and few-layers, they can undergo structural phase transformations due to dominant surface effects and show change in their electronic structure^[4]. Their ternary alloy, GaSeTe, can offer tunable structure, as well electrical and optical as properties. However, atomic structure, stacking and stability of 2D GaSeTe alloys remains an area of considerable uncertainty. In this work, we demonstrate the atomic registry of GaSeTe alloys when thinned down to mono and fewlayers (Figure 1), and reveal stacking order of multilayer crystals. In addition, we show that crystals down to 4 layers are stable and can be exfoliated in ambient environment within an hour. For isolating monolayer crystals, they have to be exfoliated in a glove box and be transferred under vacuum.

References

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Figures



Figure 1: Optical micrographs of the GaSeTe sample exfoliated onto PDMS (left) and directly transferred onto a SiN TEM grid (right). The white arrows show the location of the ultrathin GaSeTe crystal on PDMS and TEM grid.