Materials Science & Engineering Thesis Defense

Studies on Microscale Defects in Janus Monolayers

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Abstract

In the past decade, 2D materials especially transition metal dichalcogenides (TMDc), have been studied extensively due to their remarkable optical and electrical properties arising from their reduced dimensionality. A new class of materials developed based on 2D TMDc that has gained great interest in recent years is Janus crystals. In contrast to TMDc, Janus monolayer consists of two different chalcogen atomic layers between which the transition metal layer is sandwiched. This structural asymmetry induces the formation of a vertically oriented electric field or can cause strain buildup within the monolayer as a result of different electronegativity and atomic sizes of each chalcogen element. Both of the mentioned effects bring opportunities and challenges: the strong built-in electric field and the buildup of strain can lead to modification of optical and electrical properties. Nevertheless, the presence of strain brings questions regarding the synthesis of these materials, namely, at which stage strain starts to accumulate and whether it is causing defects within monolayers.

The first studies showed that Janus materials could be synthesized at high temperatures inside a CVD furnace. In that approach, the top chalcogen layer was etched by hydrogen plasma and subsequently replaced by the thermal Selenization process. Recently, a new method was proposed (selective epitaxy atomic replacement - SEAR) for room temperature Janus crystal synthesis based on plasma processing. This technique utilizes reactive hydrogen and sulfur radicals for etching and replacing top layer chalcogen atoms of the TMDc monolayer. Based on Raman and photoluminescence studies, it was shown that the SEAR method produces Janus materials of high quality. Another approach explored to synthesize Janus materials utilized pulsed laser deposition (PLD) technique. The mentioned technique uses low-energy ion implantation at moderately high temperatures (300 – 400oC) in the presence of argon gas (10-2 Torr) to replace chalcogen atoms from the top layer of TMDc monolayers. The replacement of the top chalcogen atomic layer happens in a one-step process due to its interaction with the sulfur/selenium plume.

The main scope of this work is to characterize microscale defects that emerge in 2D Janus materials after synthesizing them by SEAR and PLD techniques. For that purpose, as well as to understand the mechanism of defect formation, various microscopic techniques were used. As the main mechanism of defect formation, phenomena related to strain release were proposed. Moreover, it was shown that different positions of chalcogen atoms within the monolayer, i.e., selenium on top and sulfur on bottom or sulfur on top and Se on the bottom, lead to a distinct type of defect, e.g., the appearance of cracks or wrinkles across monolayers. In addition to the investigation of sample topography, its electrical properties were also studied by Kelvin probe force microscopy (KPFM) to observe with great precision whether the formation of defect plays a role regarding surface potential (work function). Identifying and characterizing defects and their formation mechanism in the Janus crystals is significant in understanding their fundamental properties. Further study directions have been suggested to correlate observed defects with optical and electronic properties of this material system.

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