1556
doi:10.1017/S1431927618008267
Microsc. Microanal. 24 (Suppl 1), 2018

A Review of Defects in Metal Dichalcogenides: Doping, Alloys, Interfaces, Vacancies and Their Effects in Catalysis & Optical Emission

Mauricio Terrones[1,2,3]

[1.] Department of Physics, Department of Chemistry, Department of Materials Science and Engineering and Center for 2-Dimensional & Layered Materials. The Pennsylvania State University, University Park, USA.
[2.] Institute of Carbon Science and Technology, Shinshu University, Japan.
[3.] IMDEA Materials Institute, Eric Kandel 2, Getafe, Madrid 28005, Spain and Department of Materials Science and Engineering & Chemical Engineering, Carlos III University of Madrid, Madrid, Spain.

Two-dimensional transition metal dichalcogenides (TMDs) such as MoS_2 and WS_2 hold great promise for many novel applications. Recent years have therefore witnessed tremendous efforts on large scale manufacturing of these 2D crystals. A long-standing puzzle in the field is the effect of different types of defects in their electronic, magnetic, catalytic and optical properties.

In this presentation an overview of different defects in transmission metal di-chalcogenides (TMDs) will be presented [1,2]. We will first focus on: *1)* defining the dimensionalities and atomic structures of defects (Fig. 1); *2)* pathways to generating structural defects during and after synthesis and, *3)* the effects of having defects on the physico-chemical properties and applications. We will also emphasize doping and allowing monolayers of MoS_2 and WS_2, and their implications in electronic and thermal transport. We will also describe the catalytic effects of edges, vacancies and local strain observed in $Mo_xW_{(1-x)}S_2$ monolayers by correlating the hydrogen evolution reaction (HER) with aberration corrected scanning transmission electron microscopy (AC-HRSTEM) [3]. Our findings demonstrates that it is now possible to use chalcogenide layers for the fabrication of more effective catalytic substrates, however, defect control is required to tailor their performance. By studying photoluminescence spectra, atomic structure imaging (Fig. 2), and band structure calculations, we also demonstrate that the most dominating synthetic defect—sulfur monovacancies in TMDs, is responsible for a new low temperature excitonic transition peak in photoluminescence 300 meV away from the neutral exciton emission [4]. We further show that these neutral excitons bind to sulfur mono-vacancies at low temperature, and the recombination of bound excitons provides a unique spectroscopic signature of sulfur mono-vacancies [4]. However, at room temperature, this unique spectroscopic signature completely disappears due to thermal dissociation of bound excitons [4]. Finally, hetero-interfaces in TMDs, will be studied and discussed by AC-HRSTEM and optical emission.

References:

[1] Z. Lin *et al,* 2D Materials **3** (2016), p. 022002.
[2] R. Lv *et al*, Nano Today **10** (2015), p. 559.
[3] Y. Lei *et al,* ACS Nano **11** (2017), p. 5103.
[4] V. Carozo *et al,* Sci. Adv. **3** (2017), e1602813.

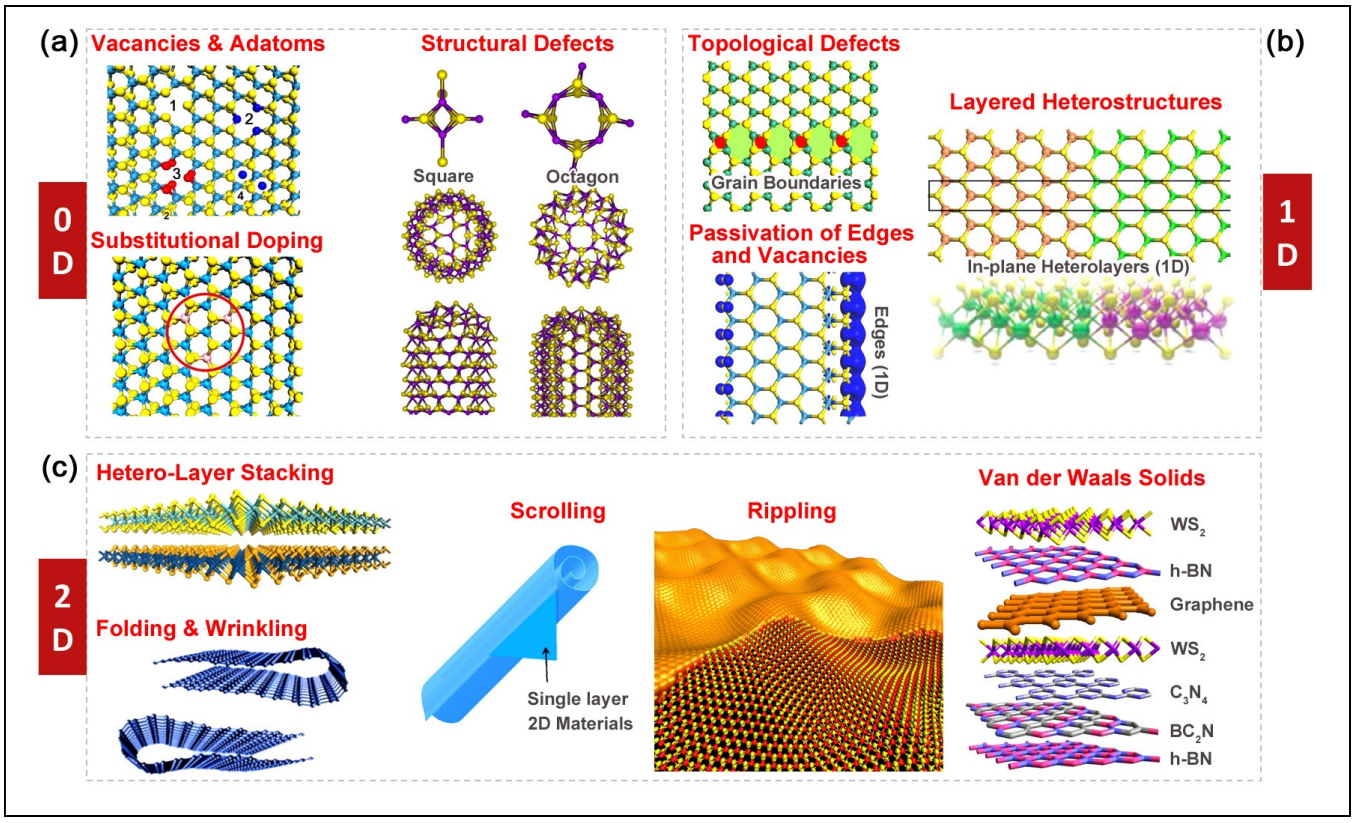

Figure 1. Different categories of defects in TMDs according to their dimensionality [1].

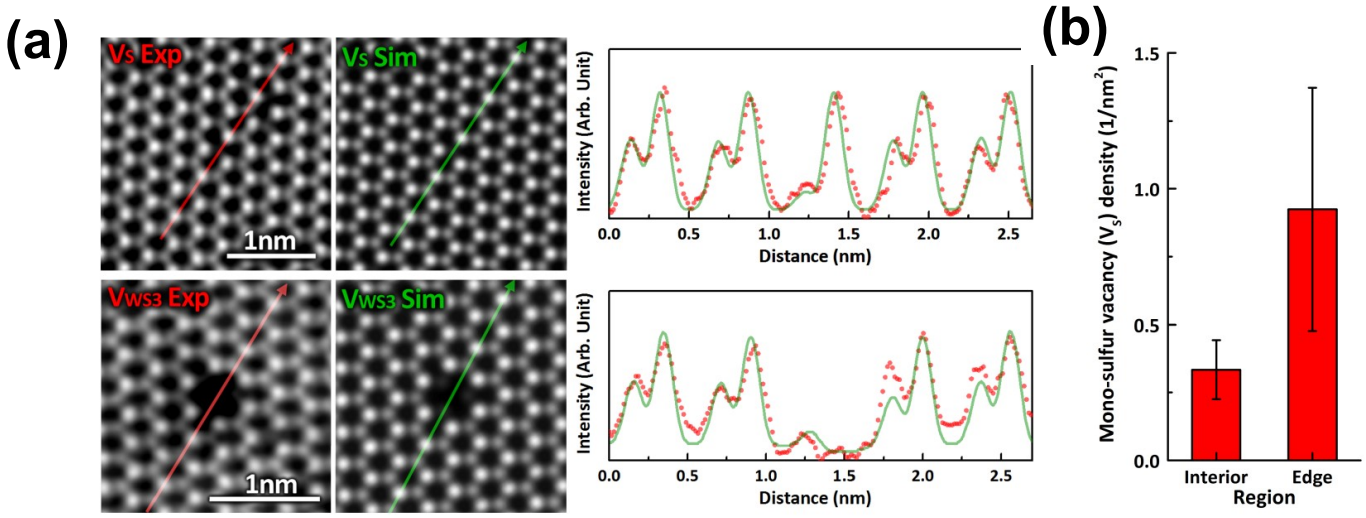

Figure 2. (a) Comparison of experimental and simulation ADF image of VS and VWS3 vacancies. The line profile was acquired along the line in ADF images. (b) Calculated monosulfur vacancy (VS) density from the center and edge regions. The error bar means SD of monosulfur vacancy density [4].

https://doi.org/10.1017/S1431927618008267 Published online by Cambridge University Press