Topotaxy in 2D materials: Towards synthesis of novel 2D materials by surface reactions

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Topotaxy is a surface reaction of deposited elements with a substrate, during which the substrate retains some structural characteristics. Such newly formed materials thus have a crystallographic relationship with the original substrate. For 2D materials, surface reactions with single molecular layers may enable their transformation into new 2D crystals. Here the potential for making new 2D materials by topotactical reactions of transition metal dichalcogenides (TMDs) with transition metals are investigated. Three distinct examples are discussed: (i) the transformation of $PtTe_2$ into Pt_2Te_2 by reaction with Pt atoms (Figure (a)) [1]; (ii) the reaction of Cr or Mn with bilayer VSe_2 to form VSe_2/Mn(Cr)/VSe_2 (Figure (b)) [2] and (iii) reaction of $MoTe_2$ with Mo to create mirror twin grain boundaries that may self-organize in periodic lattice networks (Figure (c)) [3,4]. The common concept in these surface reactions is that the reacted metals occupy ad- or ab-sorption sites which maintain a low energy van der Waals termination and thus enables the creation of new (meta) stable 2D materials. The three examples discussed here, illustrate the diversity of possible reaction products and the potential for synthesizing novel 2D materials by topotaxy.

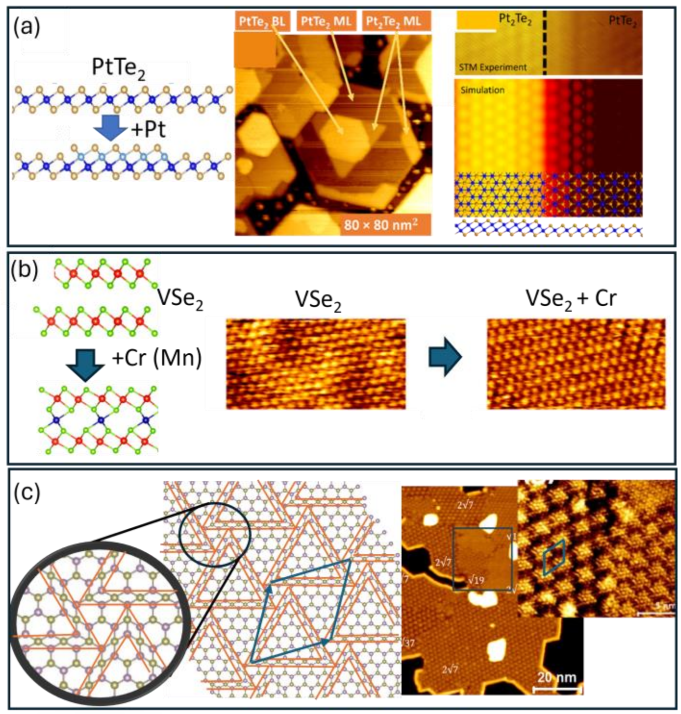

Figure: Three examples of 2D -TMDs modified by topotaxy. (a) Transformation of $PtTe_2$ to PtTe by reaction with Pt. The STM images nucleation and growth of PtTe within the $PtTe_2$ island and formation of sharp phase boundaries. (b) Intercalation of hetero-atoms (here Cr or Mn) in the van der Waals gap of VSe_2. The intercalated atoms arrange in an ordered 2×1 structure which can be identified by STM. (c) Insertion of excess Mo into $MoTe_2$ causes the formation of Mo-rich mirror-twin grain boundaries (MTBs) that can arrange into ordered networks. The STM images shows various periodicities, which vary by the length of the MTBs.

[1] K Lasek, et al. Nano Lett. 22, 9571-9577 (2022)

[2] V. Pathirage, et al. Nano Lett. 23, 9579-9586 (2023)

[3] P.M. Coelho, et al. ACS Nano 12, 3975-3984 (2018)

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