Exciton and trion emission at the edges and grain boundaries of monolayer MoS_2 grown by chemical vapor deposition

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Introduction

Thin layers of transition metal dichalcogenides (TMDCs) are in global interest as 2D materials for novel optoelectronics. Molybdenum disulfide (MoS_2) is the most studied among TMDCs. Being indirect in bulk, it possesses a direct bandgap, being only monolayer (1L) thick, and has an intense excitonic photoluminescence (PL). The PL properties can be tuned by strains in the 2D object. In particular, heterogeneous tensile strains can be initially present in MoS2 flake grown by chemical vapor deposition (CVD). Since thermal expansion of 2D MoS_2 highly exceeds that of SiO_2/Si being used as the substrate, this mismatch causes a tension of the flake when post-growth cooling. We studied PL mapping over the area of CVD-grown single- and polycrystal 1L MoS_2 flakes, focusing on trion contribution to the excitonic PL spectrum.

Results and Discussion

AFM images in Figure 1 confirm 1L thickness (about 0.7 nm) of our studied MoS_2 flakes. Raman and PL mapping show heterogeneous distribution of the spectral parameters over the flake surfaces related to tensile strains known to be present in CVD-grown material. In particular, it causes a blueshift of the Raman and PL spectra at the less strained flake edges and grain boundaries (GBs). Monitoring the PL band, a usual intensification and blue shift of the band at the flake edges and grain boundaries (GBs) between the single-crystal parts of polycrystal flakes were found. Detailed study of the PL spectral composition in Figures 2 and 3 showed that the blue shift is enhanced by a reduction of the trion (A^-) component compared to the exciton one (A^0).

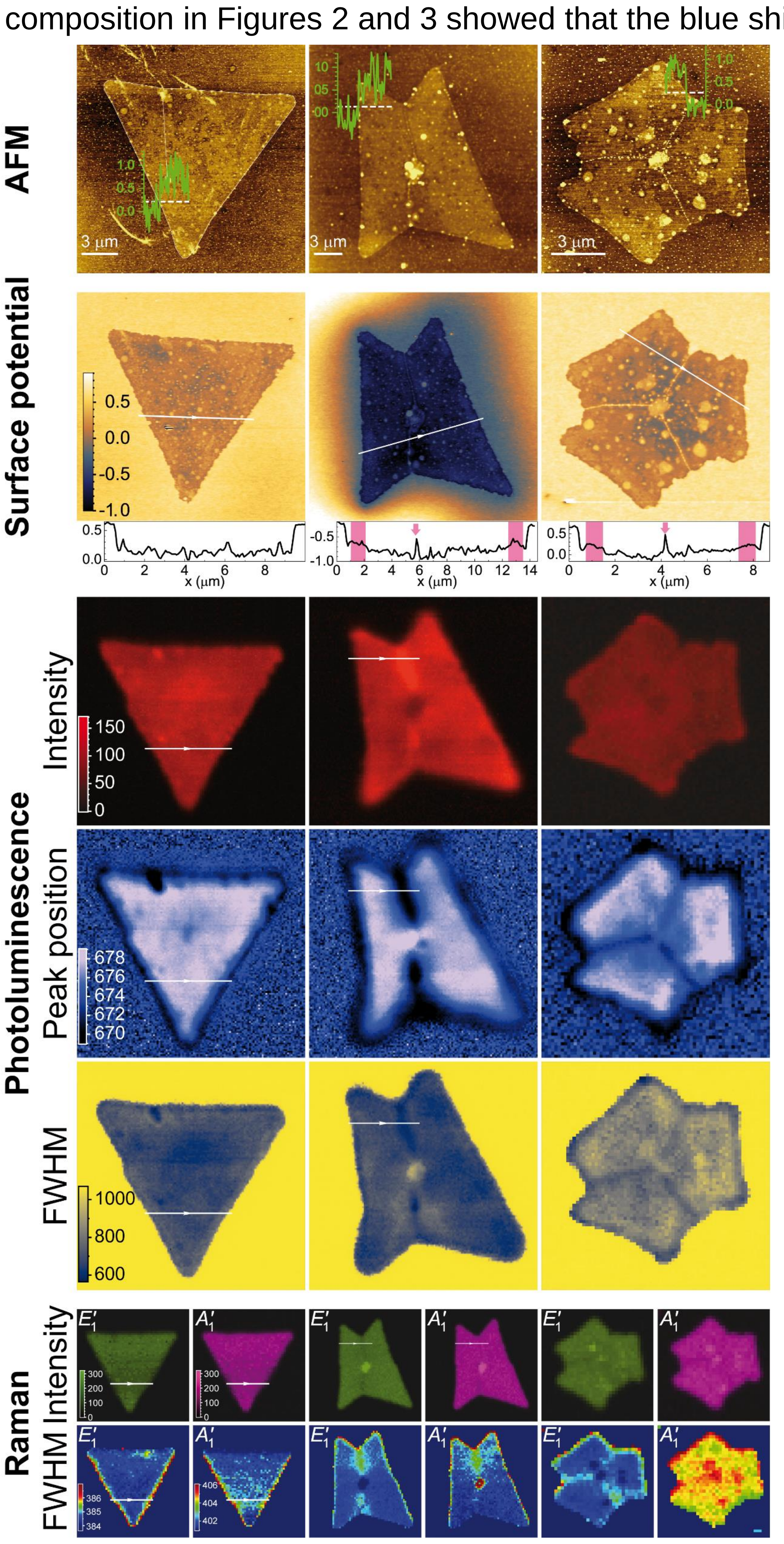

Fig. 1. AFM, Kelvin probe imaging and PL and Raman mapping of the studied 1L MoS_2 flakes. The plots under the surface potential mapping are the value distribution along the respective white lines

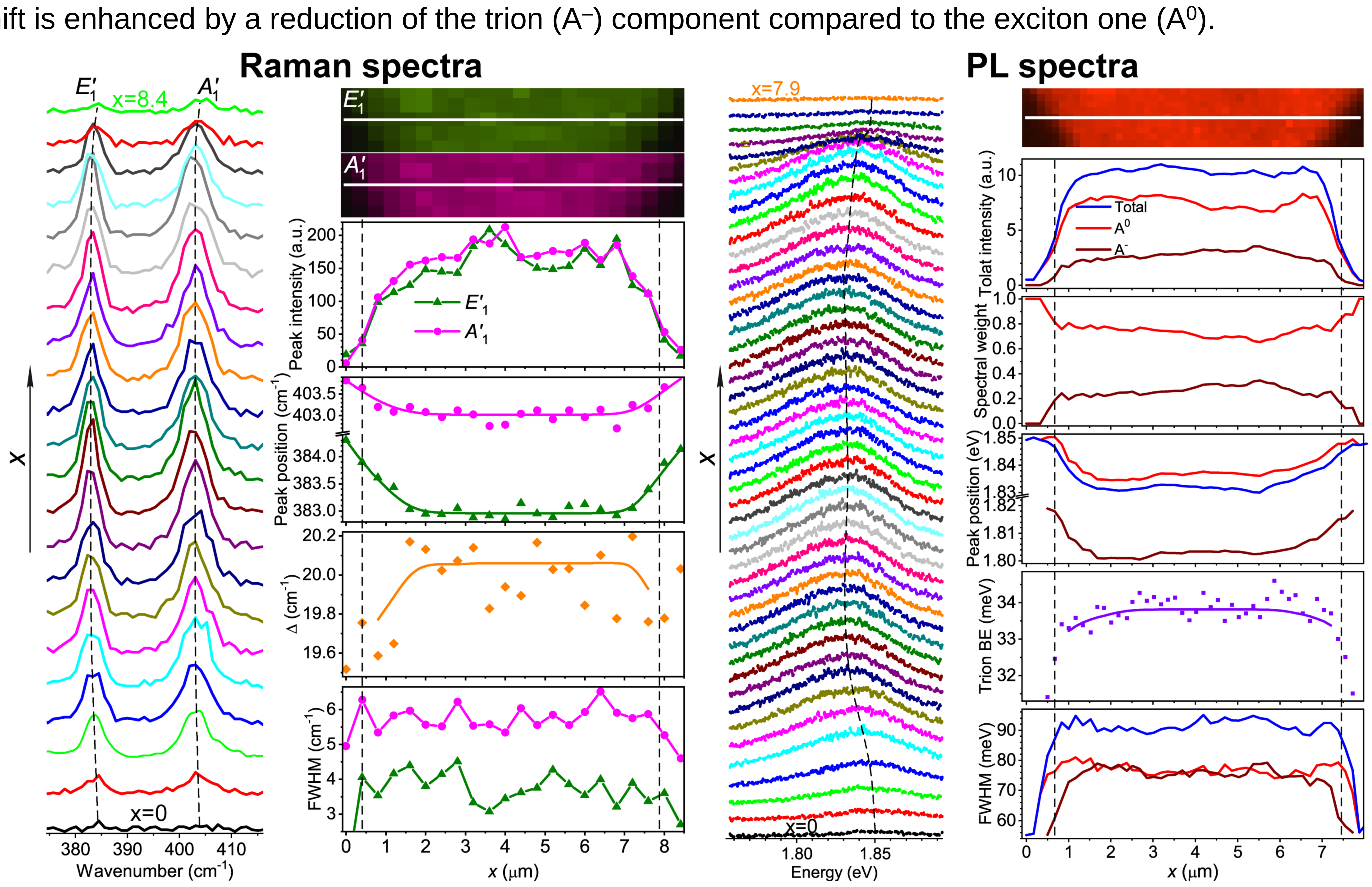

Fig. 2. Variation of the Raman (left) and PL (right) spectra of the triangle single-crystal flake along the white line in Figure 1, as well as the parameters of Lorentz peaks fitting the spectral bands. The dashed lines on the spectra show the variation of the peak positions, while the dash on the parameter plots marks the flake edges. The plot of trion binding energy was extracted as the difference between the peal positions of exciton (A^0) and trion (A^-) components.

The surface potential mapping of the samples in Fig. 1 has shown a *p*-doping at the edges and GBs, which is in accordance with the changes originated from the tensile strains and, obviously, causes a inhibition of the trion formation.

The latter contradicts to the results of other researchers that found an increase of trion at the edges and GBs along with the widening of the total PL band and attributed that to Mo-zigzag type of the edges and Mo-rich defects at the GBs, which dope the neighbor areas by electrons.

Contrarywise, we believe that our flakes have another types of the edges and GBs, that are known to be S-rich, giving an additional *p*-doping, or neutral. Thus, it provides an inhibition of the trion formation and the observed narrowing of the PL spectrum.

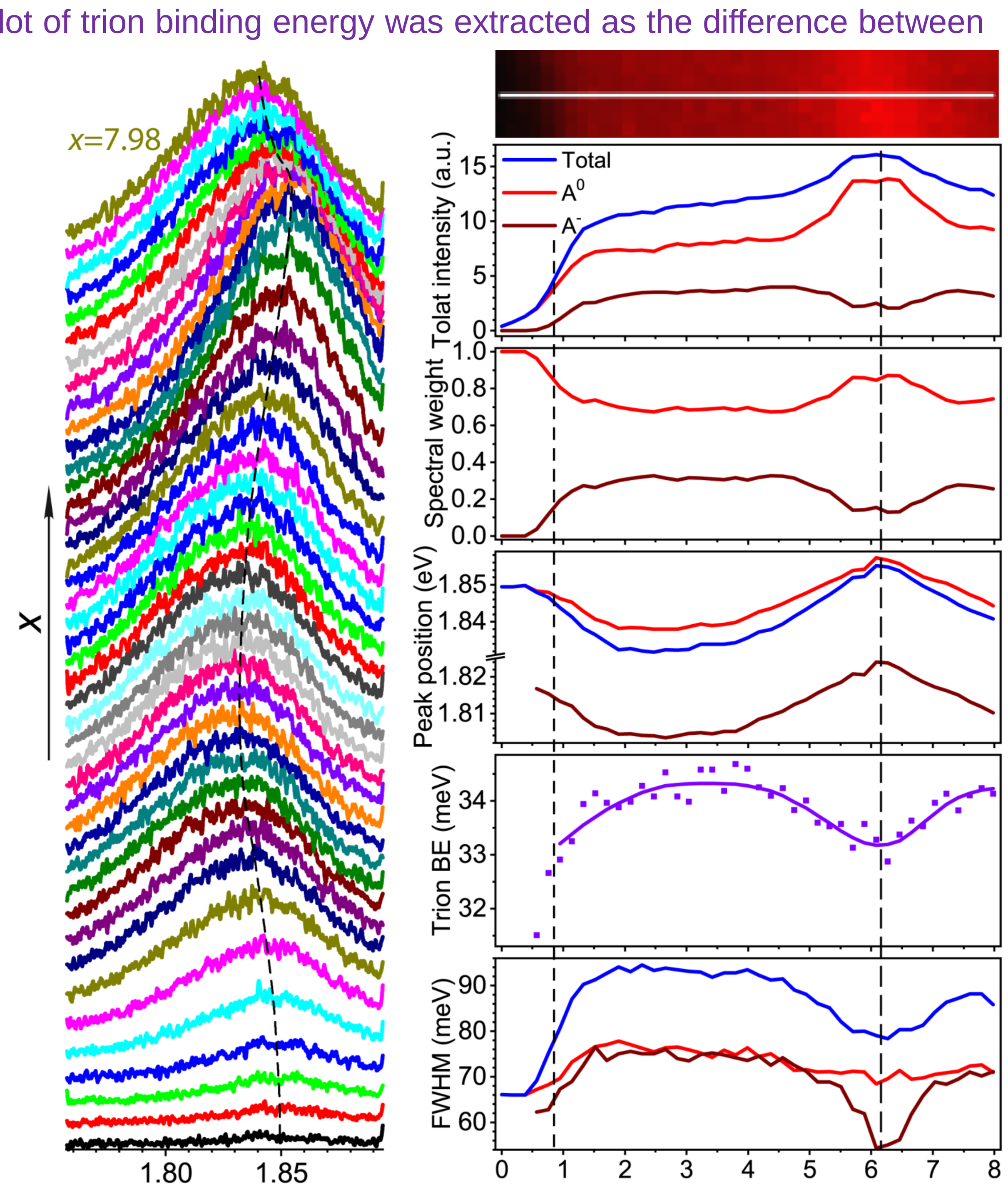

Fig. 3. Variation PL spectra of the X-like polycrystal flake along the white line in Figure 1, as well as the parameters of Lorentz peaks fitting the spectral bands. The dash on the parameter plots marks the flake edge and grain boundary.

Conclusions

The Raman and PL from the surface of 2D-MoS_2 are highly affected by the local tensile strains, which are present in the CVS-grown flakes and modify the emission properties near the edge and GBs of the flake. Also, the PL properties may be affected by the types of the edges and GBs, causing an additional doping of the areas nearby.

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