Defects and edge-related light emission of multi-layer MoS_2 studied by cathodoluminescence spectroscopy and imaging.

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Two-dimensional (2D) materials are a new type of materials under intense study because of their interesting physical properties and wide range of potential applications from nanoelectronics[1] to sensing and photonics[2]. Monolayers of semiconducting transition metal dichalcogenides MoS_2 or WS_2 have been proposed as promising channel materials for field-effect transistors. Their high mechanical flexibility, stability, and quality coupled with potentially inexpensive production methods offer potential advantages compared to organic and crystalline bulk semiconductors. An advantage of 2D metal dichalcogenides e.g. with respect to graphene is that, due to quantum mechanical confinement, the band gap of single-double monolayers of MoS_2 becomes direct in nature [3],[4]. In fact the MoS_2 emission shifts from the indirect band-gap at 1.29 eV (t> 6 MLs) to the direct band-gap at 1.8 eV (t<4 MLs). This particular effect can lead to a strong interaction with light which can pave the way for developing the next generation of visible light emitting devices.

In this work we investigate the luminescence of multi-layer MoS_2 flakes by means of cathodoluminescence (CL) spectroscopy and imaging, by comparing the optical properties of exfoliated flakes with pristine molybdenite. The structural properties of the flakes are also assessed by means of transmission electron microscopy, Raman spectroscopy and mapping. In particular, CL spectroscopy reveals a 0.75 eV emission from MoS_2 flake edges. This novel unexpected emission can pave the way of the development of MoS_2 based device for telecommunication, opening a novel scenario for this class of materials

The comparison of the room temperature CL spectra of pristine molybdenite (red line) with the MoS_2 flakes reveals that (Figure 1):

- Pristine molybednite CL spectrum shows a sharp peak at 1.25 eV, related to the indirect band-gap of MoS_2.
- The CL spectrum of exfoliated flakes presents a broad emission set at 1.08 eV and an intense emission at 0.75 eV.
- Cracked molybdenite shows mainly a strong emission around 0.75-0.8 eV

The red-shift of the indirect band-gap emission between molybdenite and exfoliated flakes (obtained from the same pristine crystal) is probably related to radiative centers caused by the formation of dislocations during the exfoliation process, as suggested by TEM investigations.

Concerning the 0.75 eV emission, its origin is still unknown since it has never been reported in the literature. However, our experimental CL results make evidence that this emission relates to states from edge surfaces or cracked crystal.

The particular edge effects are studied also by Raman mapping. Figure 2 shows that the presence of edges and dislocations in exfoliated flakes induce the inversion of the A_{1g}/E_{2g} intensity ratio, which can be then used as a probe for the presence of defects in MoS_2 flakes.

In conclusion cathodoluminescence studies reveal that the exfoliation process induces the formation of dislocations that modify the optical properties of multilayer MoS_2 flakes. In particular the indirect band-gap emission at appears 170 meV red-shifted and broaden. In addition the edges of both molydbenite and MoS_2 flakes present a new optical transition peaked at about 0.75 eV. This emission is interesting in view of developing infra-red light emitting devices for telecommunications.

References

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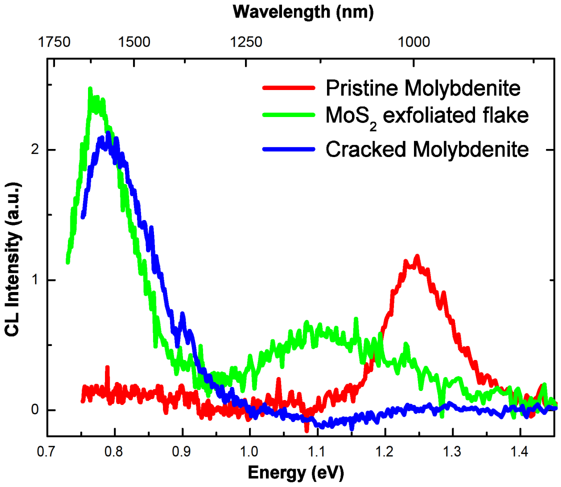

Figure 1: CL spectra of pristine molydbenite (red line), multi-layer MoS_2 exfoliated flakes (green line) and cracked Molybdenite (blue line).

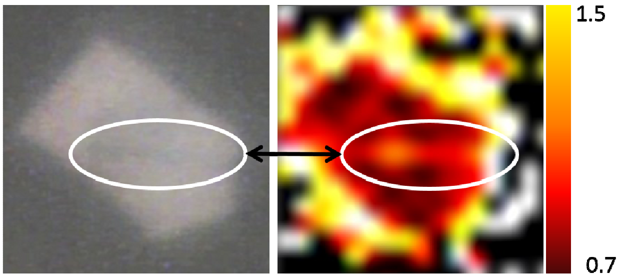

Figure 2: a) Optical image of a bulk MoS_2 flake and b) A_{1g}/E_{2g} intensity ratio map. White markers evidence the dislocation inside the flake.