Dielectric substrate and capping effects on optical properties of a few atomic monolayer MoS_2 sheets

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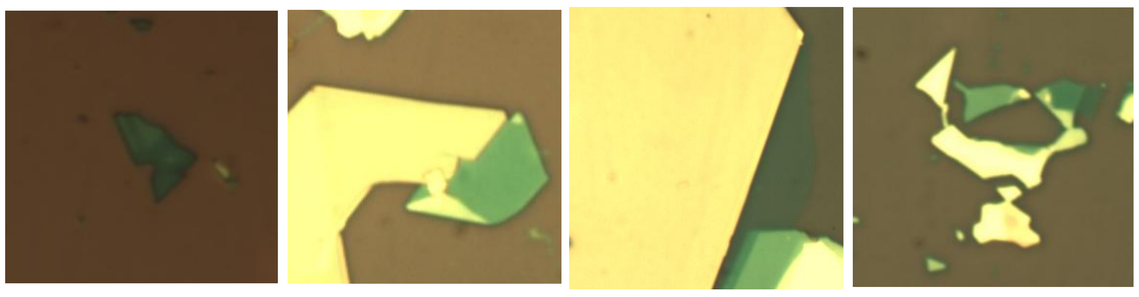
1. Introduction

✓ Molybdenum disulfide (MoS_2) is a promising layered material for the use in Field Effect Transistors.

✓ It has unusual electronic properties such as an indirect-to-direct band gap transition and strong valley polarization.

✓ Monolayer MoS_2 sheets show bright photoluminescence (PL) up to room temperature.

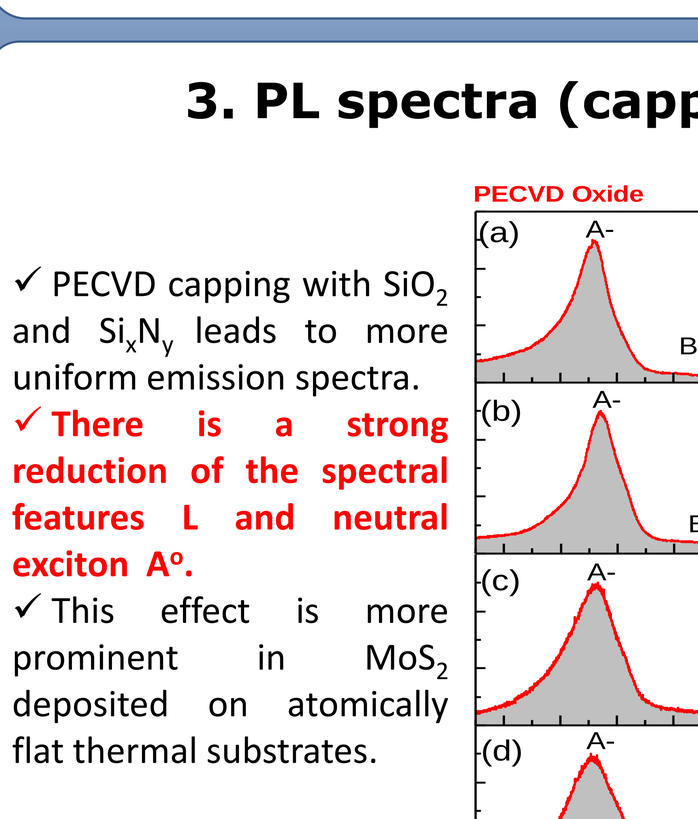
✓ **For integration of MoS_2 into devices a greater understanding of film interactions with environment is required.**



✓ This report covers MoS_2 thin films produced by mechanical cleavage and deposited on SiO_2 capped Si.

✓ MoS_2 films measured were between 2-5 atomic layers in thickness.

2. PL spectra (uncapped MoS_2)



✓ A large variation in spectral line-shape is observed reflective of differences found in the literature.

✓ Charging of the films due to interactions with the SiO_2 substrate cause the dominance of peak A- in spectra corresponding to PL of the negatively charged trion.

✓ PECVD substrates show larger contributions of L and A^0 features.

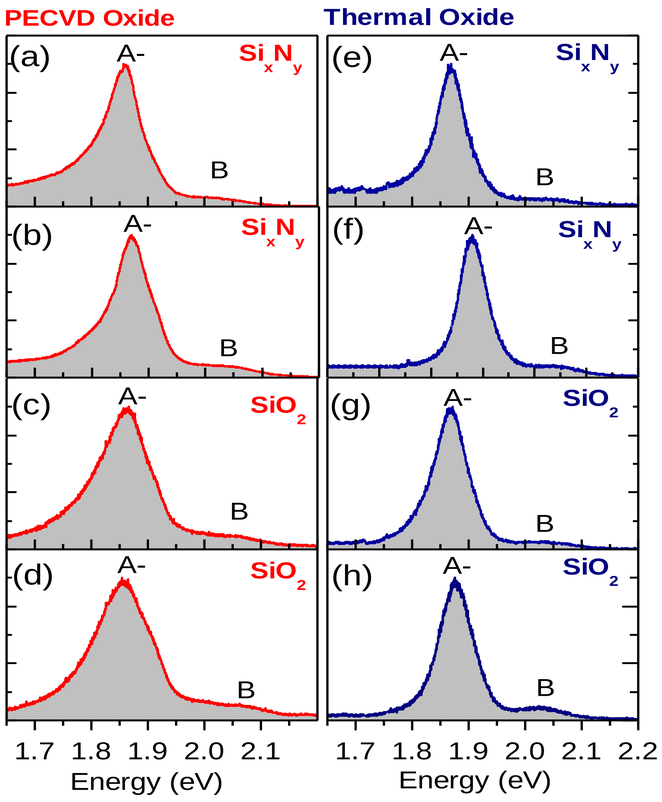
✓ **Correlation is observed between the intensities of L and A^0, with both peaks either pronounced or suppressed in a given spectrum.**

3. PL spectra (capped MoS_2)

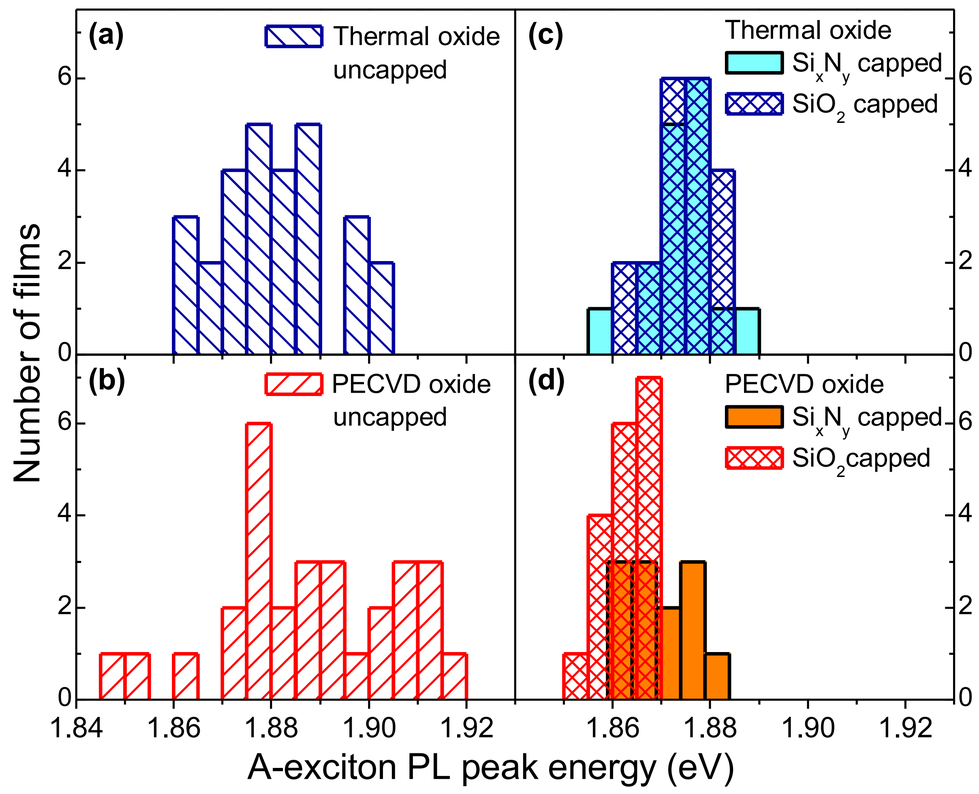
✓ PECVD capping with SiO_2 and Si_xN_y leads to more uniform emission spectra.

✓ **There is a strong reduction of the spectral features L and neutral exciton A^o.**

✓ This effect is more prominent in MoS_2 deposited on atomically flat thermal substrates.



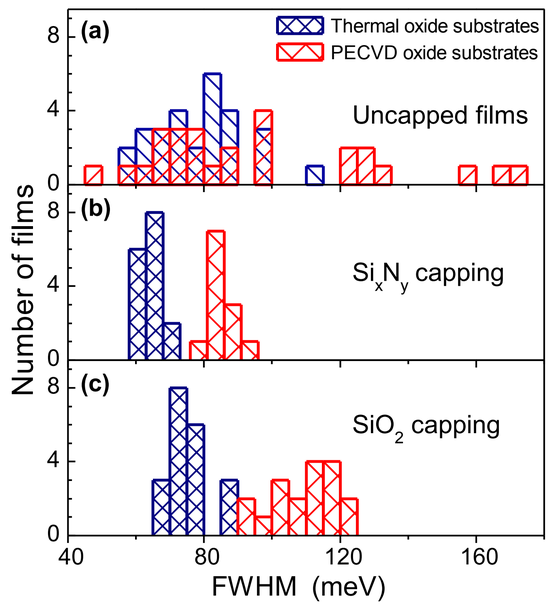
4. Effects of capping on emission energy



✓ The distribution of emission energy of the A peak is narrowed for MoS_2 sheets capped with either SiO_2 and Si_xN_y compared to uncapped sheets.

✓ A red shift up to 30 meV is observed in capped films.

5. Effects of capping on PL line-widths



✓ Capping acts to reduce the value and increase the uniformity for the FWHM of the A peak.

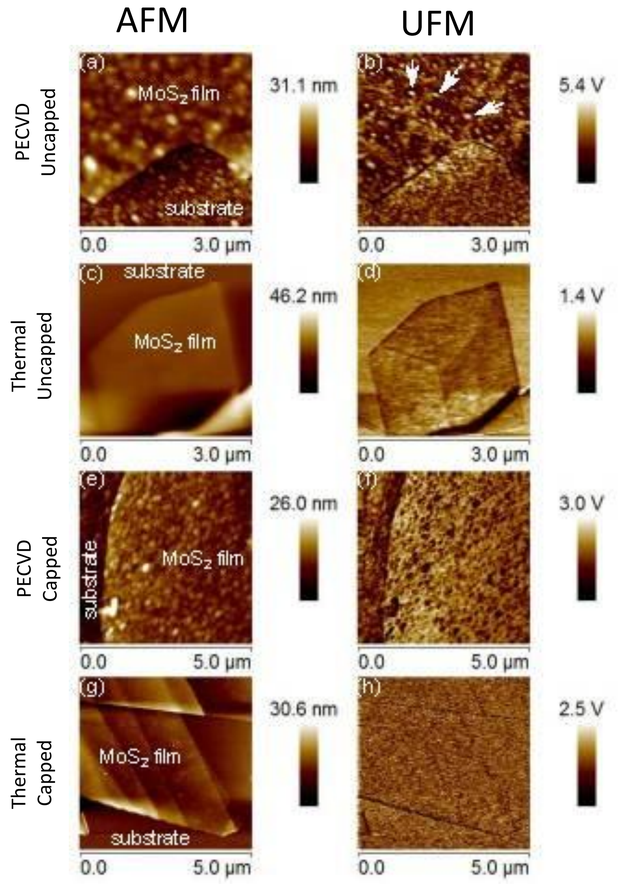
✓ **Capped MoS_2 sheets deposited on thermal oxide substrates show the narrowest line-widths.**

✓ Uncapped sheets deposited on PECVD substrates show a large variation in spectra shape, reflecting the larger contributions of L and A^0 peaks shown opposite.

6. Ultrasonic force microscopy results

✓ UFM uses an AFM tip and oscillates the sample at ultrasonic frequencies to measure the stiffness.

✓ Softer regions appear as relatively darker on images.



✓ Uncapped MoS_2 has a weak and non-uniform contact with the substrate, especially pronounced in flakes on rough PECVD substrates.

✓ The addition of a capping layer increases mechanical coupling between MoS_2 and the substrate.

✓ Mechanical coupling is strongest and most uniform for capped MoS_2 deposited on thermal substrates.

Conclusion

✓ **Mechanical coupling to surrounding dielectrics increases the uniformity of optical properties.**

✓ **When mechanical coupling is improved, MoS_2 films become increasingly negatively charged as evidenced from increased trion PL.**

✓ **Peak L is suppressed in strongly negatively charged films.**