Not just layers anymore: how Secondary Ion Mass Spectrometry reveals the chemical and structural nature of 2D material devices

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Recent advances in Secondary Ion Mass Spectrometry have enabled chemical analysis of two-dimensional materials with atomic depth resolution, as demonstrated for systems such as MoS_2[1], hexagonal boron nitride[2], and MXenes[3]. While these studies have focused on isolated materials, a natural extension is the investigation of fully functional devices, where chemical and structural complexity play a critical role. In this context, SIMS provides a unique capability to correlate local chemistry with device operation and degradation mechanisms.

This approach is particularly relevant for MoS_2-based transistors fabricated on SiO_2 substrates, whether CVD-grown or exfoliated. In CVD devices, degradation is strongly linked to the presence of sulfur vacancies, which act as active sites for chemical evolution under electrical stress. With increasing switching cycles, SIMS reveals the formation of Mo–O bonds, indicating progressive interaction between the channel and the underlying oxide. In contrast, exfoliated devices exhibit significant carbon accumulation at the Ti/MoS_2 interface, originating from transfer-related residues such as PMMA. Under repeated operation, this carbon transforms: in some cases, partial graphitization improves contact properties, while in others, redistribution and interaction with titanium lead to the formation of local Ti–C phases, increasing contact resistance and degrading device performance.

A different perspective emerges for hBN-based memristive devices, where conventional single-element analysis provides limited insight. The presence of titanium within the boron nitride layer is observed in both high- and low-resistance states, making it insufficient as a sole indicator of filament formation. Instead, a more advanced approach based on multi-atomic secondary ions is required. Species such as Ti_2, Ti_3, as well as Ti–B–Ti and Ti–N–Ti, exhibit a strong increase in intensity in the conductive state and nearly vanish when the filament is disrupted. This demonstrates that filament formation is not merely associated with elemental redistribution, but with the emergence of specific local bonding configurations that SIMS can selectively probe.

Finally, in MXene-based systems, SIMS enables spatially resolved tracking of ion transport within confined channels. Importantly, the measurements can be performed through a covering glass layer, allowing direct in situ analysis of sealed devices without the need for disassembly. By performing measurements at successive positions along the channel after ion-permeation experiments, it is possible to map the spatial decay of ion concentration and reconstruct transport profiles. This enables the extraction of effective diffusion behavior and comparison of transport efficiency for different ionic species under nanoconfinement. The observed concentration gradients provide direct insight into how ion mobility evolves with distance and confinement, linking transport properties with channel geometry and interlayer structure.

References

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