

# ToF-SIMS analyses in an H<sub>2</sub> atmosphere: Improvements in depth profiling and reduction of matrix effect

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ToF-SIMS is a very versatile and widely applicable method, but it also has its weaknesses with the most profound one being nonquantitative analysis caused by the matrix effect which also limits the capabilities of depth profiling. Namely, in SIMS depth profiling of thin films, chemically similar layers can be difficult to distinguish between each other and interfaces between them difficult to identify. The reason for this is changes in the ionization yield caused by the changes in the matrix as the chemical composition of the sample differs from layer to layer. This is the same effect that causes non-quantitative surface analysis and matrix-dependent detection limits of the same molecule or element. However, there are different ways of reducing the matrix effect. Most widely applied are laser or electron beam post ionization (SNMS), metal-assisted and matrix-enhanced SIMS, dynamic reactive ionization (DRI) and introduction of gases into the analysis chamber (gas flooding).

We applied the gas flooding approach to reduce the matrix effect and improve depth profiling results, testing different atmospheres such as H<sub>2</sub>, C<sub>2</sub>H<sub>2</sub>, CO and O<sub>2</sub> during the analysis. Only O<sub>2</sub> was previously used, while the other three gases were introduced as a novelty by our group. We achieved the best results with the H<sub>2</sub> both in the field of depth profiling and the quantitative aspect of the results measured with the mass spectra. H<sub>2</sub> atmosphere enables easier and unambiguous differentiation of layers of metals and their oxides, different metals, and alloys with different compositions. Furthermore, the identification of interfaces becomes simpler. We also did not observe a change in the sputter rate during H<sub>2</sub> flooding. [1] Surface roughening caused by the ion bombardment taking place during depth profiling was reduced in the H<sub>2</sub> atmosphere as well. This effect is more evident after sputtering a greater amount of the material and also depends on the chemical composition of the layer of interest. We assume that the most probable reason for this observation is the level of amorphization that happens during the sputtering process. [2] Our last results also show a better correlation between ratios of the SIMS signals from metals in alloys when comparing alloys with different chemical compositions analyzed in the H<sub>2</sub> atmosphere. The O<sub>2</sub> atmosphere also gives better results than UHV conditions, but improvement is less pronounced than in the case of H<sub>2</sub> flooding. These findings bring ToF-SIMS one step closer to becoming at least a semiquantitative method.

[1] J. Ekar, P. Panjan, S. Drev, J. Kovač, J. Am. Soc. Mass Spectrom., **33**, 31–44 (2022).

[2] J. Ekar, J. Kovač, Langmuir, **38**, 12871–12880 (2022).