Holistic research of the MXene phase using secondary ion mass spectrometry technique (*HoliMXene*)

One of the approaches to describing the prehistorical and historical periods, a so-called three-age system highlights the leading material that was used for manufacturing tools: Stone Age, Bronze Age, and Iron Age. Many believe that the modern times should be called Silicon Age. However, it is still debated what kind of material will play a pivotal role in the near future.

Many believe we are on the brink of the Smart Materials Age, i.e. specially designed materials that can change their properties by external stimuli. We are already using photochromic glasses which darkens on exposure to high irradiation! But we are also designing new solutions like buildings which retain the inner heat in winter and prevent heating up in summer. Or special drugs that are only released at the first sign of infection.

Interestingly, some argue that the next period should be called the Two-dimensional Materials Age. We can, however, combine these two and employ 2D materials as building blocks of larger components that can have smart properties.

MXenes – a two-dimensional form of transition metal carbides, nitrides, and carbonitrides - are the largest family of 2D materials, with over 50 representatives synthesized experimentally and many more predicted theoretically. What differentiates them from other 2D materials is their complicated structure and composition. They may consist of more than ten different elements whereas graphene or silicen contains only one, hexagonal boron nitride and molybdenum sulfide – just two.

The complex chemistry of these materials poses a significant obstacle to the precise characterization of these materials. While many techniques offer atomic spatial resolution (for example transmission electron microscopy) they lack the possibility to identify all elements, especially from the beginning of the periodic table such as hydrogen, carbon, oxygen, and nitrogen, which are very abundant in the MXene structure. On the other hand, other techniques like X-ray photoelectron spectroscopy can identify these elements but lack the spatial resolution to distinguish each atomic layer.

The current project is focused on utilizing the ultra-low-impact energy secondary ion mass spectrometry (ULIE-SIMS) technique to characterize MXenes with atomic depth resolution. The PI of the project developed the ULIE-SIMS technique to enable reaching the atomic depth resolution. Interestingly, in 2022 he showed that oxygen is incorporated in the structure of MXenes and thus these materials should be rather called oxycarbides, oxynitrides, and oxycarbonitrides. For more than ten years after the initial discovery, the scientific community was not aware of this! It pinpoints that the utilization of the technique may bring us closer to understanding, predicting, and designing further properties of these innovative materials.