

On the need of isotopically doped reference samples for atom probe tomography analyses in geoscience applications

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Atom probe tomography is a sub-nanometer analytical microscope based on time of flight mass spectrometry. Its mass resolving power (m/Dm) is about 1000, sufficient for isotope discrimination, but inefficient for isobar or mass overlaps separation. Indeed, due to the physics of field evaporation sustaining the principle of atom probe tomography, elemental species may present several charge states, resulting in overlaps between different species (for example $^{28}\text{Si}^+$ and $^{56}\text{Fe}^{2+}$, or $^{14}\text{N}^+$ and $^{28}\text{Si}^{2+}$). In addition, in the laser mode operation used for nonconductive materials, volatiles, such as H, N, C and O, may form molecular ions, making their quantification tricky. One of the options to overcome this issue, even if not widely used in the atom probe community, is the use of (minor) isotopes doping. Of particular importance for geoscience applications is the issue of oxygen quantification in mineral, as it can be detected at 16 Da as O^+ or O_2^{2+} . Resolving the atomic or molecular nature of this peak is clearly a critical issue to assess oxygen quantification. But, due to the weakness of the second natural oxygen isotope ($^{18}\text{O}=0.2\%$), it is an extremely difficult, if possible, task. The solution lies in the doping of the investigated material with ^{18}O , ideally up to 50%. As will be presented, such an approach was successfully applied to $\alpha\text{-Fe}_2\text{O}_3$ hematite [1]. We will then discuss the necessity of applying this approach to silicates or phosphates, the most common minerals, and thus of the necessity of the availability of adequate samples.

[1] M. Bachhav, F. Danoix, B. Hannoyer, J.M. Bassat, R. Danoix, Investigation of O-18 enriched hematite ($\alpha\text{-Fe}_2\text{O}_3$) by laser assisted atom probe tomography, International Journal of Mass Spectrometry 335 (2013) 57– 60

