The analysis of sulfide minerals by atom probe tomography

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Sulfide minerals, including selenides and tellurides, are of widespread interest in geology, as valuable metal ores and as geochemical reservoirs that can provide constraints on geological events and processes. They are also of interest in materials engineering, as compound semiconductors and thermo-electric materials such as HgCdTe and $(Bi,Sb)_2(Se,Te)_3$. Recently, atom probe tomography (APT) has been successfully applied to this class of materials [1-3], though limited examples have been reported for natural sulfide minerals [4].

Using a LEAP 4000X HR atom probe at the Geoscience Atom Probe facility at Curtin University, we have analysed a number of natural sulfide phases, including Pyrite (FeS_2), Troilite (FeS), Arsenopyrite (AsFeS), and Galena (PbS), as well as some telluride mineral phases such as Altaite (PbTe) and Tellurobismuthite (Bi_2Te_3). These sulfide minerals tend to field-evaporate differently from silicate and oxide minerals, usually requiring relatively low laser power, and in some cases reliably yielding large datasets under voltage-assisted evaporation.

The behaviour of these minerals in APT is important to understand in order to optimise data acquisition and obtain the best chemical quantification. Common trends are observed across the sulfides, such as increasing complexity of the time-of-flight mass spectrum, particularly with S atoms forming high-order molecular complexes under low-field conditions, and a relatively high rate of multiple-hit events at the detector. Even with 37% ion detection efficiency in the 4000X HR, the proportion of multiple-detection events can approach 80%, with this figure increasing under high-field conditions (i.e. at low laser power or in voltage-assisted mode).

This presentation will discuss the application of atom probe analysis to sulfides, including quantitative comparisons with conventional geo-analytical techniques such as TIMS and SIMS. These comparisons address critical questions surrounding the accurate chemical and isotopic quantification necessary for many geoscience applications.

The study of sulfide minerals by APT also has implications for understanding laser-assisted field evaporation of non-metallic and geological materials more broadly. Some sulfide minerals are low-bandgap semiconductors and may have significant carrier densities aided by natural impurities. Many observations are consistent with good electrical conductivity during atom probe analysis.

References:

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