

Simulated exposure of crude oil to sunlight and characterization using atmospheric pressure photoionization fourier transform ion cyclotron resonance mass spectrometry

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Petroleum is a vital resource and is likely to remain so for the foreseeable future, providing the primary basis of most transportation energy and being the precursor for many materials. Due to its finite availability, production of petroleum is in decline, although worldwide consumption continues to increase. Lower quality sources of crude oil have become increasingly exploited as a result. Releases of petroleum into the environment can occur, whether arising from natural seepage or from human activity, and it is known that natural processes can influence the chemical composition of these complex mixtures. The effects of solar radiation have been targeted for the following study.

A crude oil sample was divided into three allocations: one sample was exposed to ultraviolet light, the second sample was exposed to light from a SoLux lamp which mimics sunlight, and a third sample served as a control. After more than a month of exposure, the chemical compositions were determined and compared using a 12 T Fourier transform ion cyclotron resonance mass spectrometer.

Atmospheric pressure photoionization was selected as the ionization method due to its suitability for studying less polar components which may be present within crude oils, such as sulfur-containing compounds and hydrocarbons which do not incorporate any heteroatoms. The thousands of components observed were categorized according to heteroatom content, carbon number, and double bond equivalents, and profiles for each sample could be created. It was found that specific heteroatom classes more readily degraded, accompanied by an increase in oxygen-containing compound classes. The findings contribute to a better understanding of changes to the chemical composition of crude oil in the environment and possible changes in toxicity.

The behaviour of submicron inclusions during host deformation

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Both brittle and plastic deformation strongly influence the location, rates and mechanisms of material transport in the earth's interior. Mineral reactions and diffusion can be controlled by deformation, but in turn contribute to its localisation. We investigate the mechanisms of interaction between deformation and chemical reaction in the context of re-equilibration of inclusions in a deforming host mineral.

Permian pegmatite garnets from the Koralpe, eastern Alps, contain numerous submicron sized inclusions. The pegmatitic assemblage was affected by deformation under eclogite facies conditions during the Cretaceous tectono-metamorphic event. The meta-pegmatite garnet deformed crystal-plastically at this metamorphic stage [1].

Trails of inclusions crosscutting the garnet have a coarser grain size (1-10 μm \varnothing) than inclusions outside the trails. In 10-40 μm wide zones flanking the inclusion trails the original $\leq 1 \mu\text{m}$ sized inclusions are absent, defining bleaching zones.

FEI-microprobe data showed that it is possible to form the microstructure isochemically. However, some trails were also found where inclusions have coarsened non-isochemically. In both cases no change in garnet major element composition was observed.

From their microstructural characteristics it is inferred that the trails formed at sites of healed brittle cracks. Garnet deformation has been mapped using EBSD and correlates with re-equilibration microstructures. Bleaching zones are associated with systematic very low angle lattice rotations of garnet. Additionally, lattice rotations of up to 10° occurred adjacent to already coarsened inclusions.

The new microstructural, microchemical and textural data document several different interactions between material transport, crystallization and deformation processes which contribute to the final microstructure. TEM investigations provide the opportunity to examine the types of defects present in order to help determine the mechanisms through which chemical and mechanical processes have interacted on the nanoscale.

[1] Bestmann Et Al. (2008) *J. Struct. Geol.* **30**, 777-790.