

Mapping deformation driven chemical variation in ancient sedimentary organic matter at nanoscales with optical photothermal infrared (O-PTIR) microscopy

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Knowledge of the molecular structure of sedimentary organic matter (SOM) informs a broader understanding of petroleum generation processes as well as paleo-environments. The structure of SOM is controlled by the biogenic source material (e.g., marine vs. terrigenous), depositional environment, and thermally-driven geologic processes (e.g., catagenesis). However, geologic stress may also drive elastic and plastic strain in SOM which can affect the associated molecular structure. Most studies exploring the impact of strain on organic matter structure focus on samples from fault zones where shear stresses are very high (e.g., mylonitic coals); however, strain imparted to organic matter from deformation induced by compaction during burial may also alter the chemical makeup of these materials.

To explore the relationship between deformation and the molecular structure of SOM we have applied optical photothermal infrared microscopy (O-PTIR) to map molecular functional group distribution with 500 nm step resolution in immature *Tasmanites* (algal microfossils) from the Upper Devonian Ohio Shale. Mudstones containing *Tasmanites* represent an excellent opportunity to examine the impact of burial stress on the chemical structure of SOM as these algae are roughly spherical prior to deposition, but during burial and compaction are flattened into discoid shapes. In cross-section the flattening of the *Tasmanites* results in an elongate shape and tight folding of the algal body. Our results indicate that organic matter within the fold apices (regions of localized strain) is generally less oxygen-rich than organic matter in the surrounding *Tasmanites* body, although there are little differences observed in the hydrogen content or aliphatic branching ratios between the two regions. Observations of organic matter compositional variation between the *Tasmanites* fold apices and the microfossil body are greater for *Tasmanites* with larger surface areas. These findings indicate that strain localization due to burial stress can alter the molecular structure of SOM, although the chemical changes imparted appear minor compared to the roles that biogenic source material and thermal alteration play. Finally, this study highlights the power of O-PTIR to study SOM structure at nanoscales and this analytical approach shows great promise for future studies evaluating the molecular composition of geologic materials.

