Raman Spectroscopy

* Raman spectroscopy provides plenty of information about the rock being observed:
  + Chemical identification
  + Characterisation of molecular structures
  + Effects of bonding
  + Environment
  + Stress on a sample
* Non-destructive, up to < 1 um (high resolution)
* Diffraction-limited system - this means that because there is a principal limit to the optical properties of any instrument (due to the physics of diffraction), the system with resolution performance at the instrument’s theoretical limit is said to be diffraction-limited
* Effect of being a diffraction limited system = spatial resolution is dependent on wavelength of light and the numerical aperture of the focusing element
  + aperture = opening, hole, gap etc.
* Raman spectroscopy is a technique that provides highly chemical-specific information about samples based on the fundamental vibrational modes of the molecules
* Raman spectroscopy is used to provide a structural fingerprint by which molecules can be identified. The crystallinity index (CI) of materials can be determined via different techniques, but in raman spectroscopy, the CI is determined as the relative intensity ratio of the Raman line reflecting the amorphous and crystalline regions of materials. Can be used in the deformation of composite specimens
* Raman spectroscopy is a vibrational spectroscopic technique; vibrational spectroscopy includes several techniques, but the most important are mid-infrared (MIR), near-IR (NIR), and Raman spectroscopy. Both MIR and Raman spectroscopy provide characteristic fundamental vibrations that are used for the elucidation of molecular structure.
* While there is a limit to the vibrational frequencies observed by raman spectroscopy, sufficient information can be obtained to discriminate different structural groups or phases related to the same mineral class, like silicates or carbonates
* Sometimes high spectral resolution is needed to resolve closely spaced peaks - this is the case when specific temperature and pressure conditions are applied to recreate what can happen deep within the Earth. Spectral discrimination is key in order to detect small peak shifts induced by high temperature and pressure situations
* Raman spectral libraries are also a great help for easy identification of minerals
* **Chemical Selectivity**
  + a-Silicate minerals = silicate is a compound whose skeleton is essentially composed of silica and oxygen tetrahedra and with additional elements such as aluminum (aluminosilicates), magnesium, iron, potassium, calcium etc. They are classified by the way in which the silicate groups coalesce Diagram

    Description automatically generated
    - Raman spectra can classify particular classes of silicates

<https://www.horiba.com/fileadmin/uploads/Scientific/Documents/Raman/Geo01.pdf>

Neosilicates/Orthosilicates = Olivine

* One of the most common silicates formed by magma
* Subclass characterised by a isolated tetrahedra [SiO4]^4-
* Raman spectra shows intense stretching modes in the 800-1000 cm^-1 region and bending modes between 300 and 650 cm^-1

Inosilicates = Chain silicates = pyroxenes and amphiboles

* Amphibole - double chains of tetrahedra
  + Actinolite and its variety nephrite e.g.
* Pyroxene - single chains of SiO4

Tectosilicates = three dimensional framework silicates

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Name | Equation | Type | Raman Band | |
|  | | | Stretching Mode | Bending Mode |
| Olivine | (Mg,Fe)2SiO4 | Ferromagnesian Silicate | 800-1000 cm^-1 | 300 and 650 cm^-1 |
| Pyroxene | MgSiO3 | Ferromagnesian Silicate | 650 - 700 cm^-1 | |
| Amphibole | Fe7Si8O22(OH)2 | Ferromagnesian Silicate |  |  |
|  |  |  |  |  |

Mineral Research

* Apart from muscovite, biotite, and chlorite, there are many other sheet silicates (a.k.a. phyllosilicates), many of which exist as clay-sized fragments (i.e., less than 0.004 millimetres). These include the clay minerals kaolinite, illite, and smectite, and although they are difficult to study because of their very small size, they are extremely important components of rocks and especially of soils.Table

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Graphical user interface, table

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Faulting in Sandstones

Nicholas C. Davatzes, Peter Eichhubl, Atilla Aydin; Structural evolution of fault zones in sandstone by multiple deformation mechanisms: Moab fault, southeast Utah. *GSA Bulletin* 2005;; 117 (1-2):

* Composed of two classes of structures:
  + Deformation bands: associated with cataclastic deformation
    - Tabular zones of localised deformation that are typically charactersied by crushed grains, porosity loss and shear displacement referred to as cataclasis
  + Joints and sheared joints: represent brittle fracturing, fragmentation and brittle fracturing
    - Joints overprint deformation bands
    - Distribution is controlled by local variations in stress state that are due to mechanical interaction between the fault segments (elastic boundary model)
    - Brittle joints are planar discontinuities characterized by opening normal to the fracture plane. Joints are susceptible to reactivation in shear, which promotes the formation of new joints, called splay fractures, near the tip and oblique to the sheared joint

Fault zones for project

* 20 km Homebush Bay Fault Zone
* Faults have not moved for more than 100 million years: why?
* Non-clay gouges? Is the sample quartz cemented? Figure out cement of sample