

CRYSTALLINE DEFECTS

Most of the crystals don't have an ideal crystal lattice, they are not perfect, but contain a certain number of lattice defects, which can be caused by e.g., temperature, pressure, crystal growth, radiation or phase transitions. When numerous defects affect macroscopic properties and chemical composition of minerals, and can be responsible for a variety of phenomena such as the generation of color, diffusion, deformation processes, crystal growth, electrical resistivity or the incorporation of trace elements. Spectroscopy can be used to study such defects in minerals.

There are different types of defects, point, linear and planar, and radiation defects.

Point defects are either single atoms or clusters of atoms, extending over a few atomic diameters. They can be divided into 1) missing atoms (vacancy), 2) interstitial atoms, 3) atoms in a wrong site, or 4) impurities. Some point defects are called 'centers', originating from F-center, the german word for 'Farbzentrum', which translates as color center. Such centers are anionic vacancies. The formation of a vacancy involves a local charge readjustment to maintain neutrality in the crystal. Hence, such vacancies are filled by charge-compensating electron(s) and cause colors of minerals. If a positive ion vacancy is compensated for by a negative ion vacancy such a pair is called Schottky defect.

Alternatively a positive vacancy may be compensated by a positive interstitial nearby, which is named Frenkel defect. Another well-suited analysis technique to detect defects is transmission electron microscopy (TEM). Other types of defects are **linear defects** (e.g., dislocations) and **planar defects** (e.g., stacking faults), causing local distortions of the crystal structure, and radiation defects (observable as haloes), altering and destroying crystal structures.

To describe defects and their reactions the so-called Kröger-Vink notation is used.

What is IR spectroscopy?

IR spectroscopy is one of the most widely used and most important analytical methods in science in general. In geosciences it is a sensitive tool for mineral identification, since every mineral has a characteristic spectrum. Further applications are:

- mineral identification
- qualitative and quantitative determination of structural incorporated molecules and defects in minerals, e.g. SiO_4 , SiO_6 , PO_4 , CO_3 , OH , H_2O , CO_2
- speciation & concentration
- information about atoms and their bonds (e.g., bond distances)
- spatial orientation of dipoles

The spectral region of infrared radiation is divided into three parts:

Near-IR (NIR): 12500 - 4000 cm^{-1} — combination vibrations and overtones

Mid-IR (MIR): 4000- 400 cm^{-1} — H_2O bending and stretching vibrations

Far-IR (FIR): 400 - 0 cm^{-1} — MO_4 , MO_6 , lattice vibrations

History of IR spectroscopy

- 1800 Sir William Herschel discovered infrared radiation
- 1880 Langley introduced bolometer
- 1905 first IR spectra were published by Coblentz
- 1937 E. Lehrer first fully-automated spectrometer
- 1940 developments in USA
- 1950 well-resolved spectra
- 1946 first spectra catalogue
- 1960s introduction of Fourier Transform technique, first use of Michelson interferometer, first commercial spectrometer
- technique found much use after 1965

Source:

https://serc.carleton.edu/NAGTWorkshops/mineralogy/mineral_physics/raman_ir.html