A Very Brief Introduction to XRF Spectroscopy

Steve Kaczmarek

The geology-chemistry link

- What most people see...
  - Rocks

- What we see....
  - Geochemical Data
    - Elemental
    - Isotope
Why is geochemical data useful?

• Chemical composition of material reflects formation conditions/depositional environment
  • Elemental data – the chemistry of the environment
    • Fluid/magma composition
  • Isotope – what conditions of the environment
    • Temperature, evaporation, pressure

How do we extract geochemical data from rocks?

• Many approaches & tools in our belt
  • Atomic absorption
  • Optical emission
  • Liquid/gas chromatography
  • Mass spectrometry
  • X-ray fluorescence spectroscopy
    • Elemental composition of sample
Lecture objectives

• Understand:
• what XRF spectroscopy is,
• the basic physics of XRF,
• how XRF is used,
• limitations of XRF

Definitions

• Spectroscopy: investigation and measurement of spectra produced when matter interacts with or emits electromagnetic radiation.
• Spectra: plural form of spectrum.
• Spectrum: the entire range of wavelengths of electromagnetic radiation.

• XRF Spectroscopy: measures energy released by interactions between a sample and millions of high-energy photons
Fundamentals

- Photons emitted from source
  - Sun (infrared – ultraviolet)
  - Incandescent bulb (mostly infrared)
  - Fluorescent bulb (red – violet)
  - XRF tube (X-rays)
- Photons interact with molecules in sample
  - Reflected (white/color), absorbed (black), or scattered
- Reflected photons observed by detector
  - Eyes (red, green, blue cones)
  - XRF detector
- Information is processed
  - Brain takes information and we see color
- Source, object of interaction, & detector determine what photons can be “seen”
  - 3 sources of subjectivity
  - Everyday examples
- If variations in source and detector can be eliminated (i.e. instrument parameters controlled), then detected variations in reflected photon can be attributed to sample composition
  - This is what you do with the XRF
    - Voltage, current, time, filter, atmosphere

What’s a photon, you ask...

- Nobody really knows exactly what it is...
  - “Discrete packets (quanta) of electromagnetic radiation”
- We do have a handle on some of its properties
- No mass, but carry a force...
- Move at speed of light (c) in free space
- Can exhibit characteristics of a wave or a particle but is neither
  - Long scientific debate.....
- Slowed or absorbed when interacts with matter
- Best to think about photons in terms of a diameter
- Importantly, photons contain distinguishing information upon return to detector
X-ray fluorescence

- High-energy photons emitted from EM source
  - Rh anode (others: Cu, Mo, Cr, etc.)
  - 1 – 40 KeV (cf. ~1-3 eV visible light)
  - Higher energies can interact with the interior of the sample (cf. not just the outer layer with visible light)
    - Yields atomic information (i.e. elemental data)
• How do we know the composition?

• Periodic Table of Elements and X-ray Energies
What is recorded by the detector

**Analysis of Spectra**

Spectra = frequency histogram

The x axis shows increasing energy - each element ‘lights up’ at a different and unique energy

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**The Physics**

High-Energy Photon Source
Photon-Sample Interaction

Photon interaction with sample produces “fluorescence”

- Ejected K-shell electron
- (1/7) M-shell electron fills vacancy
- (6/7) L-shell electron fills vacancy
- Kα x-ray emitted
- Kβ x-ray emitted

Ejected photons hit detector & specific energies are recorded

- 140 eV-resolution Si-drift detector
Emitted photons hit detector & specific energies are recorded

- 140 eV-resolution Si-drift detector

How XRF is used by geoscientists

- Identify elements of interest (economic minerals)
  - Gold, silver, copper
- Identify proxy elements (indicators of special environments/conditions)
  - Mo, Ti, U
- Identify changes in mineralogy
  - E.g., clays, quartz, calcite, dolomite, gypsum, pyrite
- Looks for systematic trends spatially and temporally (stratigraphically)
  - Changes
- Be sure to visit the student posters
Advantages & Limitations

- Non-Destructive
- Liquids, solids, and thin films
- Sample Prep: minimal
- Rapid and inexpensive
- Easy, but requires understanding

- New tool in geological studies
- Matrix effects common
- Calibration needed
- Sample variables
- Health considerations

Hazards of X-rays

- X-rays are energetic electromagnetic radiation that ionize matter by ejecting electrons from atoms
- Ionizing radiation deposits energy at the molecular level, causing cellular chemical changes, and thus biological changes. Damage is not caused by heating, but by molecular changes.
- The extent of ionization, absorption, and molecular change depends on the quality (spectral distribution) and quantity (flux & intensity) of the radiation.
Summary

• Geochemical data is critical for geoscientists
• XRF is one of many tools to extract elemental data
• XRF spectroscopy works by shooting high-energy EM at a sample and recording the energy released during electron interactions
• The energies of the returning EM depend on the elemental composition of the sample

Additional Resources

• [http://www.xrf.guru/](http://www.xrf.guru/)