EDX Spectra Simulation in EPMA
Optimisation of Excitation Conditions, Calculation of Detection Limits
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Principles of EPMA / EDX Spectra Simulation

The accuracy of database is crucial for quality of simulation

- All line- and binding energies
- Relative emission rates in a single shell
- Excitation of sub-shells
- Coster-Kronig transitions
- Fluorescence yields

Standardless absolute calculation of X-ray excitation processes

- Characteristic- and Bremsstrahlung radiation excitation (cross sections)
- Absorption of X-rays (excitation depth)
- Fluorescence and other effects

Simulation of detector effects and statistics

- Escape-effect and artefacts
- Resolution and peak shape effects
- Pulse statistics

Standardless determination of absolutely calculated concentrations (Pb-based) is applicable and proven since a decade and more. It works without normalisation to 100 per cent and without any information in addition to the spectrum, except the excitation conditions (ED, geometry) and detector parameters. The simulation of EPMA spectra is simply the inverse procedure of this real standardless spectrum evaluation. The fundamental parameter based absolute Pb-ratio calculation and a reliable simulation of Bremsstrahlung over the entire distribution of energies are the basics for the simulation of spectra. In contrast to Duncumb and Statham (1), the local Pb-ratio (Bremsstrahlung of same energy) is used.

Application and Benefits of Spectra Simulation:

MA-Table simulation program examples

Optimisation and verification before spectra acquisition:

- Variation of primary electron energy (E0)

The peak-position shifts because of:

Lxx (L-shell)

Lx (subshell)

Lxx (subshell)

Estimation of detection limits (MDL)

- Variation of specimen tilt angle

5% Pd in Lead

Comparison with real measured spectra:

- Gives answers to questions:
  - Are there additional elements?
  - Need to improve database?

Determination of Minimum Detection Limits (MDL) is always based on Pb-ratios. That is why the expected MDL can be calculated in advance, if an absolute Pb-determination algorithm is used.

More info and download:
www.microanalyst.net

References: