Problems in Trace Element EPMA: Modeling Secondary Fluorescence with PENEPMA

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In EPMA the incident electron beam scatters, producing the "electron interaction volume". However, X-rays produced within that volume may spread tens to hundreds of microns and produce secondary fluorescence in other materials. This can be ignored in many/most cases where major element compositions are being measured. However, when minor or especially trace elements are being measured by EPMA, secondary fluorescence needs to be considered. In some cases it can be eliminated by separating the materials and mounting them by themselves, or by reducing the kV to minimize fluorescence. However, in many cases these efforts are not possible. In those cases, modeling the EPMA experience by Monte Carlo simulation is useful. PENEPMA is a Fortran program based upon the PENELOPE radiation transport model of Salvat et al (2006). It differs from other MC electron interaction programs in that it follows each electron and photon and records all interactions at each point in the "particle's path". It also permits complicated geometries with many materials. Both continuum and characteristic secondary fluorescence can be tracked, and at the end of a run, compared to x-rays produced only from primary electrons. This has important applications in geology and petrology. Llovet and Galan (2003) used it to correct calculations for olivine-cpx thermobarometry. Recent attention has been given to Ti in zircon as a geothermometer. PENEPMA has now been used to model 2 different situations: (1) rutiles present on or near zircon, (2) ilmenite present near zircon. In the first case, several geometries are modeled: a 30 micron diameter zircon (Ti-free) is surrounded by Ti-bearing silicate glass (yielding an apparent 452 ppm Ti in zircon core); with five 30 um surrounding rutiles at 15 micron distance (yielding an apparent 948 ppm Ti in zircon core); if the silicate glass were replaced by epoxy, the apparent Ti would increase to 1179 ppm. In a second case, the effect of zircon with nearby ilmenite in a rock was simulated by a simple 2-slab geometry. PENEPMA shows that at 10 um distance into the zircon there would be ~1000 ppm Ti by secondary fluorescence, gradually reducing to ~100 ppm at 40 um distance. Note that in both cases the issue is continuum fluorescence. Uncorrected EPMA measurements would yield incorrectly high temperatures using the Ti-in-zircon thermometer.

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