

**s5.m1.o1** **HRTEM contribution to the reactivity of rock-forming silicates.** A. Baronnet, *CRMC2-CNRS, Campus Luminy, Case 913, 13288-Marseille cedex 9, France.*

Keywords: electron crystallography, mineralogy.

Transmission electron microscopy of minerals at high resolution documents mostly retrograde transformations in rocks. When metamorphic and igneous rocks cool down, ongoing mineral reactions are incipient and fine-grained products are located within, or close to, prograde phase boundaries.

Combined high resolution transmission electron microscopy imaging (HRTEM), selected area electron diffraction (SAED), and analytical electron microscopy (AEM) provide invaluable informations about the reaction mechanisms at the quasi atomic scale. This works when the mother phase(s) and the daughter phase(s) coexist, i.e. for reactions arrested before completion at some closing temperature.

At low solid/fluid ratios, the dissolution / crystallization mechanisms predominate whereas high solid/fluid ratios favour solid-state transformation mechanisms. In the latter case, coexisting species display tight crystallographic relationships (topotaxy) which largely illustrate the principle of saving the nature and/or orientation of structural modules of silicates as far as possible. Metastable structural states often come in between mineral reactants and products. The oxygen framework is virtually unaffected during most reactions. Such structural inheritance is more frequent than maintenance of local chemistry. This indicates that microstructures might be more efficient than chemical composition in tracing back the history of a rock. However several reaction mechanisms coexist frequently side-by-side for one and the same mineral system. It is not clear in many cases whether they were simultaneously used by Nature or were operating successively during the cooling of the host rock.

The above conclusions will be illustrated mainly from hydrothermally altered and/or hydrothermally grown silicates: pyroxenes, amphiboles, biopyriboles, planar and rolled layer silicates, and their association.

**s5.m1.o2** **Structure determination from electron diffraction intensities: practical applications in materials science.** J. Gjønnes, V. Hansen and K. Gjønnes, *Center for Materials Science, University of Oslo, Gaustadalleen 21, N-0349 Oslo, Norway.*

Keywords: electron crystallography, mineralogy.

Quantitative electron crystallography has emerged as a viable option for determination of crystal structure of materials, as well as an important addition to the characterization techniques offered by the transmission electron microscope. Why, when and how to use these options? The aim of the talk is to outline some methods and their practical applications in materials science.

Ways to collect better and more extensive intensity data is a key factor: recording by imaging plates or slow-scan CCD instead of film; convergent-beam diffraction (CBED), or precession scanning as alternatives to the selected area or micro-diffraction modes; procedures for merging electron diffraction intensities into three-dimensional sets data sets. It is shown that structure solutions can be derived from such data by standard crystallographic programs assuming kinematical scattering, even in cases where dynamical scattering effects are appreciable. Which means that the statistical relations behind direct methods are to a large extent preserved.

As a further development approximate expressions of dynamical scattering theory has been incorporated in the statistical direct methods taken over from x-ray crystallography. Intensities collected by the precession technique are treated as 'quasi two-beam' and used to derive 'dynamical structure factors'. Next step is to determine the true structure factor amplitudes and signs by an iteration procedure. Alternative approaches are based on CBED-profiles and an iterative *ab initio* determination of structure factor amplitudes and phases.

Examples to be discussed are intermetallic phases found in aluminium alloys. Emphasis will be on practical approaches: collection of intensity data, merging to a three-dimensional set, assignment of space group from CBED and Patterson maps, confirmation of structure solution, crystallographic characterisation of materials, and combinations with other methods, *e.g.* powder diffraction.