European Mineralogical Conference
Vol. 1, EMC2012-611, 2012
European Mineralogical Conference 2012

Thermal Expansion Tensor Calculating and Three-dimensional thermal Expansion Diagrams Drawing: software "High temperature expansion tensor determination for crystalline materials – ThetaToTensor (TTT)"

R. Bubnova (1,2), V. Firsova (1), and S. Filatov (2)

(1) Institute of Silicate Chemistry of the RAS, (2) Saint Petersburg State University, Geological Faculty, Crystallography Department, St. Petersburg, Russian Federation (rimma_bubnova@mail.ru)

A detailed knowledge of the crystal structure at elevated temperatures has several potential applications to mineralogical as well as geophysical researches. Oblique-angle minerals such as feldspars, many amphiboles, pyroxenes, and micas, due to high anisotropic thermal expansion are responsible for the decompression of the rocks that they compose, as well as for increases in rock permeability by fluids and in some cases for the accumulation of ores under metamorphic conditions. Similarly, sharply anisotropic thermal expansion of calcite is responsible for the thermal decompression of marbles and for the location of some ore deposits in the marbles.

Here we present the software developed to determine thermal expansion tensor for minerals as well materials with any crystal system using experimental powder low- and high-temperature X-ray diffraction data. The realized algorithm gives it possible to do the determinations from diffraction Bragg angles calculations to expansion tensor 3D-drawing with tensor and crystallographic axes oriented in physical coordinate system. The software includes the programs of diffraction data processing, 2 Theta calibration with standard, calculation of unit cell dimensions at different temperatures, approximation of unit-cell temperature dependencies using polynomial and power functions, determination of expansion tensor parameters and its orientation in coordinate axes. Initial data and computed results are displayed in 2- and 3-dimensial format.

This software can be used for investigations of thermal expansion anisotropy of crystal materials and phase transitions. The crystal symmetry imposes limitations on the thermal expansion tensor. Minerals of oblique angle crystal systems (monoclinic and triclinic) occupy a special place. In this case, the problem associated with determination of the principal axes orientation. Due to its calculation most of oblique-angle minerals exhibit sharply anisotropic thermal expansion including contraction (negative expansion) along some directions. Examples are given.