

**Experiment title:**

Equation of state of 3T-phengite from high temperature and high pressure powder diffraction data

Experiment**number:**

HS-346

Beamline:

ID30

Date of experiment:

from:22.10.97

to:26.10.97

Date of report:**20.02.98****Shifts:**

15

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Report: Micas are sheet silicates where one occupied octahedral sheet (O) and two tetrahedral (T) sheets form TOT layers, linked one another by K or Na cations. The presence of several cations both in octahedral (mainly Mg/Al) and in tetrahedral (Si/Al) independent sites causes order/disorder phenomena to occur, which strictly are related to the stability of polytypes, originated by different stacking of layers. A sample of phengite 3T from the Dora Maira Massif (western Alps) $[(K_{0.90}Na_{0.01})(Ti_{0.01}Al_{1.43}Mg_{0.58})(Si_{3.57}Al_{0.43})O_{10}(OH)_2; a=b=5.214, c=29.738 \text{ \AA}]$, previously proved to bear both tetrahedral and octahedral cation order by neutron diffraction (Pavese et al, 1997), has been investigated, at high temperature and pressure, by means of powder X-ray diffraction, at ESRF Facility, to determine its EOS. Measurements were performed on the ID30 beamline ($\lambda=0.2451 \text{ \AA}$), over the range $0 < P < 6 \text{ GPa}$ and $300 < T < 1000 \text{ K}$, by means of a Paris-Edinburgh-like cell. Pressure and temperature were gauged by internal calibrant (NaCl) and Pt-thermocouple, respectively. The spurious effects due to the conditioning chamber have been discarded by subtracting, at each P-T point, the environmental pattern (i.e. that from the cap enveloping the sample) from that bearing the diffraction signals from phengite. The cell parameters have been extracted from the diffraction patterns by multi-phase profile analysis according to the LeBail et al (1988) method, as implemented in the GSAS software package (Larson and Von Dreele, 1986),

from a total of 90 profiles, measured along 8 isotherms, by 0.5 GPa steps. P-V-T data have been interpolated through a Vinet-like EOS (Vinet et al, 1987), which presently is one of the most flexible function for exploring the thermobaric space. The results achieved by this treatment have further been compared with those obtained using the Birch-Murnaghan (1986) EOS, along each isotherm. On the basis of this analysis, the thermoelastic properties of phengite 3T can be summarized as follows (B:bulk modulus, B' : its first derivative vs P; α :thermal expansion):

$B=54.4(2.9)$ GPa, $B'=8.3(1.8)$, $\alpha=35(2) 10^{-6} \text{ K}^{-1}$, in keeping with inferences from high pressure powder neutron diffraction measurements (experimental report submitted -ISIS), yielding $B=56.4(4.0)$ GPa, $B'=5.6(2.3)$, and from high temperature data (Pavese et al, 1997), indicating $\alpha=33 10^{-6} \text{ K}^{-1}$. In Fig.1 the RT-raw profile (sample+environment+internal standard) at 3.3 GPa is reported.

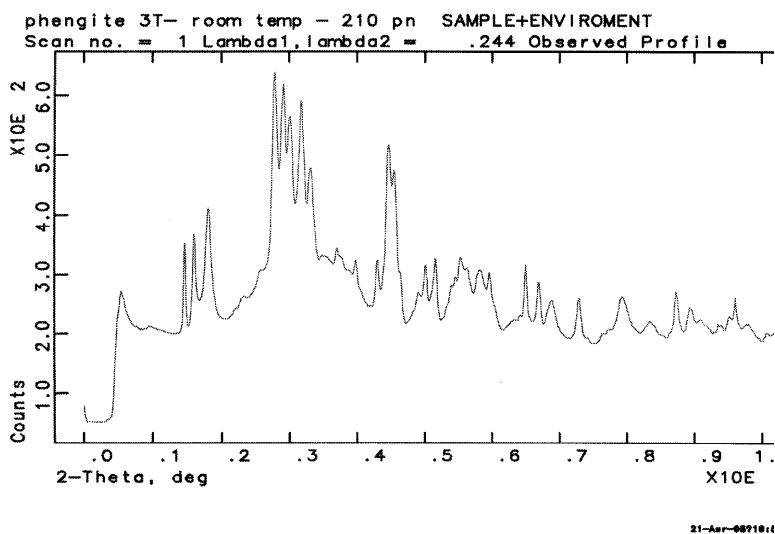


Fig.1

References

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