American Mineralogist, Volume 109, pages 243–254, 2024

Thermal and combined high-temperature and high-pressure behavior of a natural intermediate scapolite

Paolo Lotti[1,*,‡], G. Diego Gatta[1,†], Lara Gigli[2], Hannes Krüger[3], Volker Kahlenberg[3], Martin Meven[4], Davide Comboni[1,5], Sula Milani[1], Marco Merlini[1], and Hanns-Peter Liermann[6]

[1]Dipartimento di Scienze della Terra, Università degli Studi di Milano, Via Botticelli 23, 20133, Milano, Italy
[2]Elettra Sincrotrone Trieste S.c.P.A., Strada Statale 14-km 163.5 in AREA Science Park, 34149 Basovizza, Trieste, Italy
[3]Institut für Mineralogie und Petrographie, Leopold-Franzens Universität Innsbruck, Innrain 52, 6020 Innsbruck, Austria
[4]Institut für Kristallographie, RWTH Aachen, and Jülich Centre of Neutron Science at the Heinz Maier-Leibnitz Zentrum, Lichtenbergstraße 1, 85748 Garching, Germany
[5]European Synchrotron Radiation Facility, 71 Avenue des Martyrs, CS40220, 38043 Grenoble Cedex, France
[6]Deutsches Elektronen-Synchrotron DESY, Notkestrasse 85, 22607 Hamburg, Germany

Abstract

A natural intermediate member of the scapolite solid solution {Me_{47}; chemical formula: $(Na_{1.86}Ca_{1.86}K_{0.23}Fe_{0.01})(Al_{4.36}Si_{7.64})O_{24}[Cl_{0.48}(CO_3)_{0.48}(SO_4)_{0.01}]$}, with the unusual *I*4/*m* space group, has been studied at various temperatures and combined high-*T* and high-*P* by means of in situ single-crystal and powder X-ray diffraction, using both conventional and synchrotron X-ray sources. In addition, single-crystal neutron diffraction data were collected at ambient-*T* and 685 °C. A fit of the experimental *V*-*T* data with a thermal equation of state yielded a thermal expansion coefficient at ambient conditions: $\alpha_{V25°C} = 1/V_0 \cdot (\partial V/\partial T)_{P,25°C} = 1.74(3) \cdot 10^{-5}$ K^{-1}. A comparative analysis of the elastic behavior of scapolite based on this study and previous high-*T* XRD data suggests that a thorough re-investigation of the different members of the marialite-meionite solid solution is needed to fully understand the role of crystal chemistry on the thermal behavior of these complex nonbinary solid solutions. The experimental data obtained within the full temperature range of analysis at ambient pressure confirm that the investigated sample always preserves the *I*4/*m* space group, and possible implications on the metastability of *I*4/*m* intermediate scapolite are discussed. Neutron diffraction data show that no significant Si and Al rearrangement among the *T* sites occurs between 25 and 685 °C. The combined high-*T* and high-*P* data show that at 650 °C and between 10.30(5) and 10.71(5) GPa a phase transition toward a triclinic polymorph occurs, with a positive Clapeyron slope (i.e., d*P*/d*T* > 0). A comprehensive description of the atomic-scale structure deformation mechanisms induced by temperature and/or pressure, including those leading to structural instability, is provided based on single-crystal structure refinements.

Keywords: Scapolite, temperature, pressure, phase transition, synchrotron X-ray diffraction, neutron diffraction; Microporous materials: Crystal-chemistry, properties, and utilizations