X線回折法と計算機シミュレーションによるシリカクラスレート鉱物の相転移の研究

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X-ray diffraction and niolecular dynamics studies of the phase transitions in selica clathrote miuerals

Research Project

Project/Area Number

12640466

Research Category

Grant-in-Aid for Scientific Research (C)

Allocation Type

Single-year Grants

Section

一般

Research Field

Petrology/Mineralogy/Science of ore deposit

Research Institution

Kanazawa University

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Research Abstract

1. The structure of low melanophalohite was firstly determined using specimens from Mt. Hamilton (Ca), and thenrefined with intensity data measuread on a 4-circle diffractometer. The low form, which is a superstructure of the high temperature cubic one, results in the first order phase trasition from the cubic form.
2. The structural changes in a wide range of temperature from -50 to 200℃ were studied with X-ray single crystal techniques, showing the trasition point at about 70℃. Si-O distances and Si-O-Si angles, both for the atomic mean positions, show a begative correlation : Si-O decreases significantly in the range of the low form, while Si-O-Si increases.
3. Some of oxygen atoms show remarkable anisotropy in atomic mean swuare displacements, suggesting a possible disorder.

4. The maximum entropy method was applied to analyze electron density distribution in the high form, indicating that all the cages of pentagon dodecahedron are occupied by CH4, which are possibly in six oreintations.
5. Melanophlohite releases its guest molecules at a temperature as high as 1000℃. The guest-free specimen obtained by heating up to 1000℃ belongs to the cubic space group as the same as that of natural specimens, and show no structural transition with varying temperatures. This result denies a reported one based on a NMR study.
6. Some trials of MD simulations for a model structure with pentagon dodecahedral cages, fully occupied by CH4 molecules, succeeded to reproduce the structure transition from the cubic form to the (2x2x1) tetragonal superstructure. This suggests that guest molecules play important roles in the structural transitions in melanophlogite.

Research Products (10 results)

All Other

All Publications

[Publications] Kuniaki Kihara: "Molecular dynamics interpretation of structural changes in quartz"Phys. Chem. Minerals. 28. 365-376 (2001)

[Publications] Kuniaki Kihara: "Thermal expansions in quartz : a geometrical consideration"J. Miueralo. Petrolo. Sciences. 96. 159-163 (2001)

[Publications] T.Nakagawa: "The crystal structure of low melanophlogite"Amer. Mineral.. 86. 1506-1512 (2001)

[Publications] 木原國昭: "SiO_2多形の結晶構造と相転移について"日本結晶学会誌. 43. 218-226 (2001)

[Publications] 木原國昭: "SiO_2多形と構造転移"岩石鉱物科学. 31. 38-41 (2002)

[Publications] Yasuhiro Shimada: "An X-ray diffraction study of shock-wave densified SiO_2 glasses"Phys. Chem. Minerals. (in press). (2002)

[Publications] K. Kihara: "Molecular dynamics interpretation of structural changes in quartz"Phys. Chem. Minerals. 28. 365-376 (2001)

[Publications] K. Kihara: "Thermal expansions in quartz : a geometrical consideration"J. Mineralo. Petrolo. Sciences.. 96,No.4. 159-163 (2001)

[Publications] T. Nakagawa, K. Kihara, K. Harada: "The crystal structure of low melanophlogite"Amer. Min.. 86. 1506-1512 (2001)

[Publications] Y. Shimada, M. Okuno, Y. Shono, M. Kikuchi, K. Fukuoka, and N. Ishizawa: "An X-ray diffraction study of shock-wave densified Si0_2 glasses"Phys. Chem. Minerals. (In the press). (2002)

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