

石英及び関連物質の相転移: X線単結晶解析とラマン分光法による研究

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1996 Fiscal Year Final Research Report Summary

Structure transitions in silica minerals-a joint atudy of X-ray diffraction and computer simulation

Research Project

Project/Area Number

07640637

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

Principal Investigator

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Project Period (FY)

1995 - 1996

Keywords

silica mineral / structure transition / computer simulation / X-ray diffraction / quartz / berlinite

Research Abstract

This study has been projected to establish the atomic views about the mechanism of structure transition and fluctuation of related physical properties in quartz and its isostructural compounds, by combinatorial application of diffraction and spectroscopic techniques. Although two years were not long enough to perform all the projected subjects, especially spectroscopic experiments, several powerful computer programs were developed to analyze

position-time data provided by usual molecular dynamics calculations.

Detailed crystal structure analyzes of AlPO₄ and GaPO₄, both having the quartz type structures, were also completed for single crystal intensity data obtained at different temperatures.

The software package CRYSTAL has five program-units, SDSTR, MDPDF, ORDERP, DTRANS and NOMODE, each executed by teading in data from MD calculations, to calculate scattering intensities (for neutron or X-ray diffraction), dynamical structure factors, atomic probability density functions, atomic mean-square displacements, order parameters and finally normal mode analysis (still under development), respectively. In application of these programs to the MD results for berlinite AlPO₄, an order-disorder type mechanism was found to play important role in the alpha-betastructure transition in this mineral. This result is so important and still preliminary at present, but is not consistent with recent studies such as X-ray results (by the present author), hyper Raman results and hard mode infrared absorption results and so on. The results of the MD calculations must be examined for their reliability, and then some long-term calculations for MD are currently undertaken.

Research Products (12 results)

All Other

All Publications (12 results)

- [Publications] S. Kitchin, S. Kohn, R. Dupree, M. Henderson & K. Kihara: "In-situ ²⁹Si MAS NMR studies of structural phase transitions of tridymite" Amer. Mineralogist. 81. 550-560 (1996) ▼
- [Publications] Y. Muraoka & K. Kihara: "The temperature dependence of the crystal structure of berlinite, a quartz-type form of AlPO₄" Phys. Chem. Minerals. (Accepted). (1996) ▼
- [Publications] H. Okudera, K. Kihara & T. Matsumoto: "Temperature dependence of structure parameters in natural magnetite : Single-crystal X-ray studies from 126 to 773K" Acta Crystallographica. B52. 450-457 (1996) ▼
- [Publications] H. Nakae, K. Kihara, M. Okuno & S.Hirano: "The crystal structure of the quartz-type form GaPO₄ and its temperature dependence" Zeit. fur Krist.210. 746-753 (1995) ▼
- [Publications] K. Kihara: "Disorder and successive structure transitions in the tridymite forms of SiO₂" Phys. Chem. Minerals.22. 223-232 (1995) ▼
- [Publications] K. Kihara: "Temperature dependence of crystal structure data obtained in X-ray structure analyses and its application to studies of the quartz type structures (In Japanese)" Chikyuu Monthly. 12. 142-147 (1995) ▼
- [Publications] S.Kitchin, S.Kohn, R.Dupree, M.Henderson and K.Kihara: "In-situ ²⁹Si MAS NMR studies of structural phase transitions of tridymite" Amer. Mineralo.81. 550-560 (1996) ▼
- [Publications] Y.Muraoka and K.Kihara: "The temperature dependence of the crystal structure of berlinite, a quartz-type form of AlPO₄." Phys. Chem. Minerals. (Accepted). (1996) ▼
- [Publications] H.Okudera, K.Kihara and T.Matsumoto: "Temperature dependence of structure parameters in natural magnetite : Single-crystal X-ray studies from 126 to 773K" Acta Crystallographica. Vol, B52. 450-457 (1996) ▼
- [Publications] H.Nakae, K.Kihara, M.Okuno & S.Hirano: "The crystal structure of the quartz-type form GaPO₄ and its temperature dependence." Zeit. Fur Krist.210. 746-753 (1995) ▼
- [Publications] K.Kihara: "Disorder and successive structure transitions in the tridymite forms of SiO₂" Phys. Chem. Minerals. 22. 223-232 (1995) ▼
- [Publications] K.Kihara: "Temperature dependence of crystal structure data obtained in X-ray structure analyzes and its application to studies of the quartz type structures (In Japanese)" Chikyuu Monthly. 12. 142-147 (1995) ▼

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