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

Research Project

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Research Category

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Allocation Type

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Section

一般

Research Field

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Research Institution

Kanazawa University

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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 AlPO_4 and GaPO_4, 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 AlPO_4, 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^<29>Si 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 AIPO_4" 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 GaPO_4 and its temperature dependence" Zeit. fur Krist.210. 746-753 (1995)

[Publications] K. Kihara: "Disorder and successive structure transitions in the tridymite forms of SiO_2" Phys. Chem. Minerals.22. 223-232 (1995)

[Publications] K. Kihara: "Temperature dependence of crystal structure date obtained in X-ray structure analyses and its application to studies of the quartz type structures (In Japanese)" Chikyuu Monthly. 12. 142-147 (1995)

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