

Dynamical structure analyses of phase transitions and physical properties in minerals

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Dynamical structure analyses of phase transitions and physical properties in minerals

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鉱物学(含岩石・鉱床学)

Research Institution

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Dynamical structure analysis / Crystal structure / Phase transition / Lattice dynamics / Debye-Waller factor / quartz type structure

Research Abstract

In this study, X-ray diffraction data obtained in accurate structure analyses of some common minerals such as quartz and its related materials were interpreted in conjunction with lattice dynamical calculations of phonon frequencies. The chief results are summarized below.

1. Anisotropic Debye-Waller factors of atoms in quartz obtained in normal structure analyses were reproduced in lattice dynamical calculations with sufficient agreement. This agreement strongly supports that the alpha-beta phase transition is rather displacive.
2. The cusp-shape anomaly of the Debye-Waller factors of atoms in quartz, which were previously found around the alpha-beta transition, was found to be caused not only by the optic soft mode, but also by the low frequency acoustic mode in the 00xi direction.
3. The alpha-beta transition in AlPO₄, which has the quartz-type structure, is also displacive.
4. Diffraction data such as anisotropic temperature factors of atoms can be a useful candidate in analyzing dynamics of structures, in conjunction with lattice dynamical calculations.

Research Products (12 results)

All Other

All Publications (12 results)

[Publications] Kuniaki Kihara: "The temperature dependence of the anisotropic mean-square displacement of atoms in quartz" Acta Crystallogr.A46. PS-07.03 (1990) ▼

[Publications] Kuniaki Kihara: "An X-ray study of the temperature dependence of the quartz structure" European Journal of Mineralogy. 2. 63-67 (1990) ▼

[Publications] Kuniaki Kihara: "Lattice dynamical calculations of anisotropic temperature factors of atoms in quartz, and the structure of β-quartz" Physics and Chemistry of Minerals. (1992) ▼

[Publications] 木原 國昭: "格子力学計算による石英の原子の異方性温度因子" 日本結晶学会誌. 34. 249-254 (1992) ▼

[Publications] Masaaki Okuno: "The structure of (Na_{0.5}Ca_{0.5})Ga_{1.5}Ge_{2.5}O₈ and CaGa₂₀ glasses" Mineralogical Journal. 15. 64-72 (1990) ▼

[Publications] Hideshi Fujishita: "Crystal structure and phase transitions of intermediate phase of PbZrO₃" J.Phys.Soc.Japan. 61. 3606-3612 (1992) ▼

[Publications] Kuniaki Kihara: "The temperature dependence of the anisotropic mean-square displacement of atoms of atoms in quartz" Acta Cryst.A46. ps-07.03. (1990) ▼

[Publications] Kuniaki Kihara: "An X-ray study of the temperature dependence of the quartz structure" Europ. Journal of Mineralogy. 2. 63-67 (1990) ▼

[Publications] Kuniaki Kihara: "Lattice dynamical calculations of anisotropic temperature factors of atoms in quartz, and the structure of beta-quartz" Physics and Chem. of minerals. (1992) ▼

[Publications] Kuniaki Kihara: "Lattice dynamical calculations of anisotropic temperature factors of atoms in quartz (In Japanese)" J. of Cryst. Soc. of Japan. 34. 249-254 (1992) ▼

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