Crystallography

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Electron density distribution in alpha silicon nitride through synchrotron powder diffraction data

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Introduction

Silicon nitride is an important ceramic material because of its excellent mechanical properties, thermal stability, wear resistance and corrosion resistance at high temperatures. There exit two polymorphisms of alpha and beta silicon nitride. The alpha silicon nitride belongs to the hexagonal space group $P31c$ and its crystal structure has been investigated by some researchers. However, the electron density distribution in alpha silicon nitride has not been known yet. The purpose of this study is to investigate the electron-density distribution in the alpha silicon nitride using the synchrotron powder diffraction data.

Experiment

Synchrotron powder diffraction experiment was conducted using the multiple-detector system installed at the beamline BL-4B2 of the Photon Factory, KEK, Japan. Monochromatized 1.2049Å X-ray was used for the diffraction experiment. The diffraction data was analyzed by Rietveld method. with computer program RIETAN-2000. The electron-density distribution was studied by a maximum-entropy method (MEM) using the structure factors obtained in the Rietveld analysis. The calculation was performed by a computer program PRIMA with 78×78×56 pixels in the hexagonal lattice.

Results and discussion

Structure refinements of alpha silicon nitride were successfully performed assuming the space group P31c. Unit-cell parameters were refined to be a=b=7.7519(2) Å, c=5.6196(1) Å, alpha=beta=90 deg and gamma =120 deg.

In the refined structure, a Si atom is coordinated tetrahedrally by four N atoms and one N atom is coordinated by three Si atoms. It was confrmed that the crystal structure of alpha silicon nitride has two layers of AB and CD. The MEM density map indicates a covalent bonding between Si and N atoms (Fig.1)

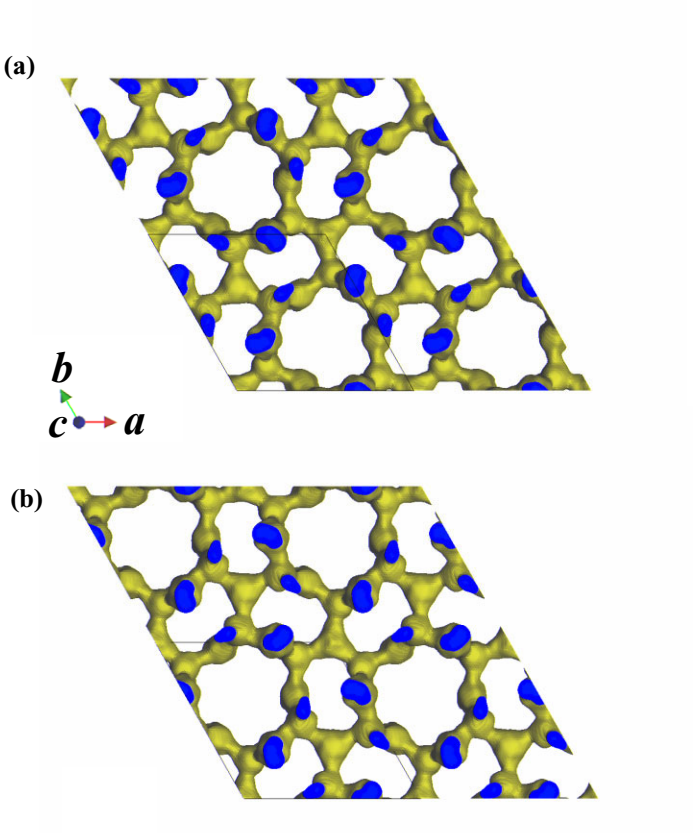

Figure 1. Equidensity surfaces at 0.8 e/Å^{-3} of electron density on the a-b plane of alpha silicon nitride. (a) AB layer ($0.32 \leq z \leq 0.82$) and (b) CD layer ($-0.18 \leq z \leq 0.32$). Solid line stands for the unit cell of the alpha silicon nitride.