

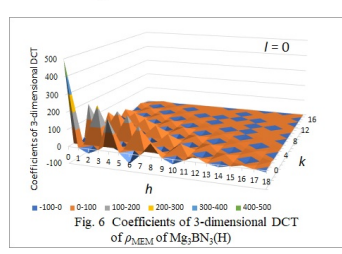
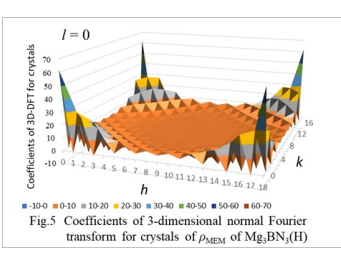
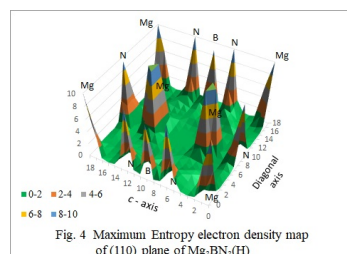
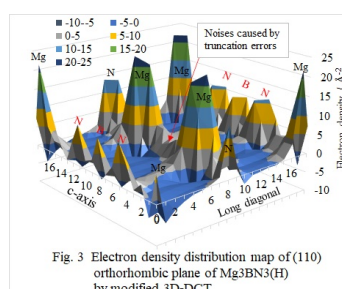
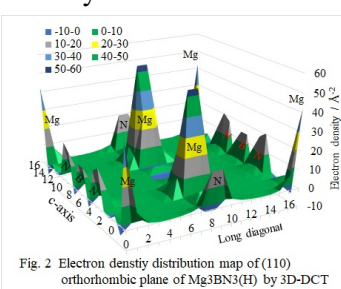
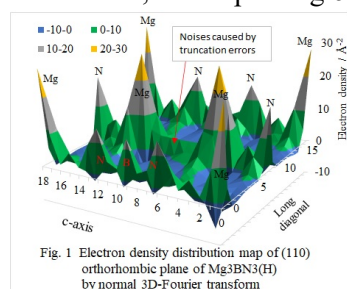
Comparative Study of Electron Density Distribution Maps and Crystal Structure Factors of Mg_3BN_3 High Pressure Phase by Discrete Cosine Transform and Maximum Entropy Method

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It is known that the electron density distribution maps calculated by the normal Fourier transform have noises caused by truncation errors as shown in Fig.1. The Maximum Entropy method can be used to eliminate the noises by the truncation errors as shown in Fig.4. In this research, it has been found out that the 3-dimensional DCT⁵⁾ can diminish the truncation errors of the electron density distribution maps of the center symmetric crystals such as $\text{Mg}_3\text{BN}_3(\text{H})$ ^{1)~3)} (Space group : Pmmm Orthorhombic) as shown in Fig.2⁴⁾. For these calculations, $Fhkl$ ($h=0\sim 8$, $k=0\sim 8$, $l=0\sim 8$) and $19\times 19\times 19$ voxels in the unit cell were used. Though there is no bonding electrons between Mg atoms, the noises exist in the region in Fig.1. Meanwhile, there are no electrons in the region of the 3D-DCT map in Fig.2. However, the modified 3-dimensional DCT cannot diminish the truncation errors as shown in Fig.3. To compare the coefficients between the normal Fourier transform and the DCT, the coefficients were calculated respectively as shown in Fig.5 and Fig.6. The map in Fig.5 has a symmetric center. Meanwhile, the map in Fig.6 has no symmetric center.



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