Ability of Electron Density Calculation via Three Dimensional Discrete Cosine Transform for Crystallography

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It is known that electron density distribution maps of crystals can be drawn via the three-dimensional discrete cosine transform (3D-DCT). However it isn't well known that how precisely the 3D-DCT can calculate the electron densities of crystals. Therefore, in this research the height of electron densities of Mg3BN3 high pressure phase (Mg3BN3(H) Space group : Pmmm Orthorhombic) of various number of voxels was calculated to confirm the precision of the ability of 3D-DCT. For these calculations, Fhkl (h=0~8, k=0~8, l=0~8) and 18×18×18 to 306 ×306×306 voxels in the unit cell were used. As a result, it turned out that the value of the height of the electron density of Mg at the origin position of the unit cell approaches the theoretical value 74.2 / Å-3 (B =1) at more than almost 144×144×144 voxels in Figure 1.

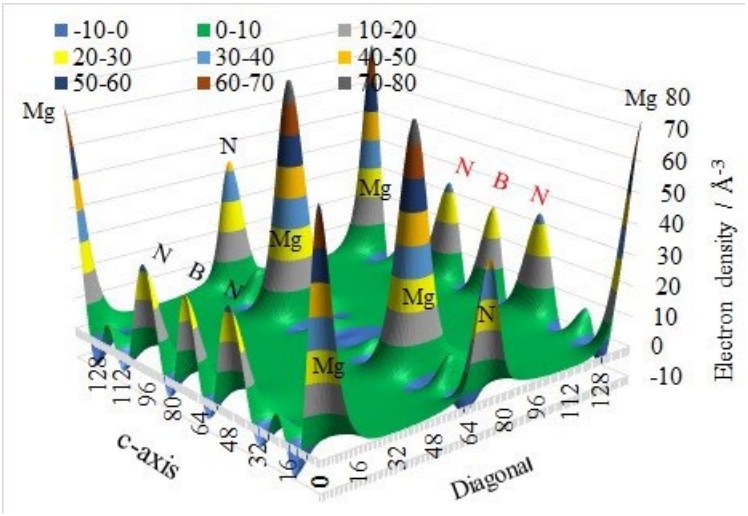

Figure 1: Electron density distribution map of (110) Orthorhombie plane of Mg3BN3(h) by 3D-DCT