Electron densities of Mg$_3$BN$_3$ high pressure phase calculated via three – dimensional discrete cosine transform incorporated into maximum entropy method

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Electron densities of Mg$_3$BN$_3$ high pressure phase (Mg$_3$BN$_3$(H), $a$=3.0933, $b$=3.1336, $c$=7.7005 Å, Pmmm, Orthorhombic) have been obtained by using the 3–dimensional discrete cosine transform (3D-DCT) incorporated into the Maximum Entropy method (MEM) in Fig. 1. This new estimation method is used for only mirror symmetric structures with a centre of symmetry. The crystal structure of Mg$_3$BN$_3$(H) is a mirror symmetric structure. Therefore, this method is suit for Mg$_3$BN$_3$(H). In this calculation, theoretical $F_{hkl}$ ($h=0$–$4$, $k=0$–$4$, $l=0$–$4$) obtained by using VESTA and 73×73×145 voxels in the unit cell were used. For the starting electron densities to execute the Maximum Entropy method, the 3D-DCT electron densities whose negative electron densities were replaced for 0.1/Å$^{-3}$ were used. This calculation was performed until the constraint function $C$ became smaller than 1. As shown in Fig. 2, the electron density of Mg is 61/Å$^{-3}$, which is near to the theoretical value 74/Å$^{-3}$. Because the 3D-DCT electron density of Mg is 38/Å$^{-3}$, the estimated electron density of Mg obtained by the 3-D DCT incorporated into the Maximum Entropy method is nearer to theoretical value 74/Å$^{-3}$ than the 3D-DCT electron density. When using theoretical $F_{hkl}$ ($h=0$–$8$, $k=0$–$8$, $l=0$–$8$) whose $h$, $k$, $l$ are larger than 4, the 3D-DCT electron density of Mg is about 72/Å$^{-3}$, which is extremely near to the theoretical value. Therefore, even though the theoretical $F_{hkl}$ ($h=0$–$4$, $k=0$–$4$, $l=0$–$4$) whose $h$, $k$, $l$ are smaller than 8 is used for the electron density calculation, the estimated electron densities are nearer to the theoretical electron density values. When the number of observed $F_{hkl}$ is smaller, this point is an advantage of this novel estimation method via the 3D-DCT incorporated into the Maximum Entropy method. Moreover, the short computational time is an advantage, too. Comparison of the shapes of the electron density curves between the Maximum Entropy method incorporating the 3D-DCT and the normal Maximum Entropy method is the next challenge, because some results have begun to be obtained that the electron density curve shape of the former method is more rounded than that of latter one.

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**Figure 1.** Electron densities of (110) surface of Mg$_3$BN$_3$ (H) via Maximum Entropy method incorporating 3D-DCT started from DCT results.

**Figure 2.** Comparison of electron densities of Mg$_3$BN$_3$(H) via DCT and MEM incorporating 3D-DCT started from DCT results


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