New Electron Density Distribution analysis of Mg_3BN_3 High Pressure Phase and Low Pressure Phase via Modified Three-Dimensional Discrete Cosine Transform and Maximum Entropy Method

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The previous researches[1),8)] have shown that the precise electron density distribution of Mg_3BN_3 high pressure phase (Mg_3BN_3(H), Orthorhombic Pmmm) which has both a center of symmetry and planes of symmetry can be calculated via the Maximum Entropy method[6),7)] incorporating the normal 3-dimensional Discrete Cosine Transform[5)] (3D-DCT) (Fig. 1). However, because Mg_3BN_3 low pressure phase (Mg3BN3(L)[2)-4)]) has a center of symmetry and a glide plane, the modified 3D-DCT[5)] is needed to calculate the electron density distribution. Therefore, in this research, the electron density distribution of Mg_3BN_3(L) (Fig. 3) has been calculated via the Maximum Entropy method incorporating the modified 3D-DCT by using a starting normal 3D-DCT map whose negative electron densities were replaced by 0.001 $Å^{-3}$ (Fig. 2).

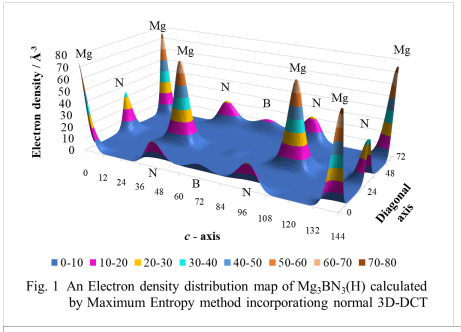

Fig. 1 An Electron density distribution map of Mg_3BN_3(H) calculated by Maximum Entropy method incorporationg normal 3D-DCT

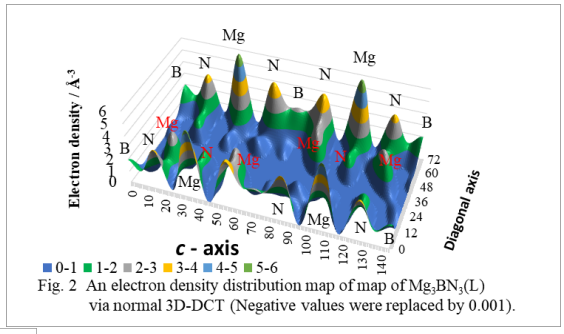

Fig. 2 An electron density distribution map of map of Mg_3BN_3(L) via normal 3D-DCT (Negative values were replaced by 0.001).

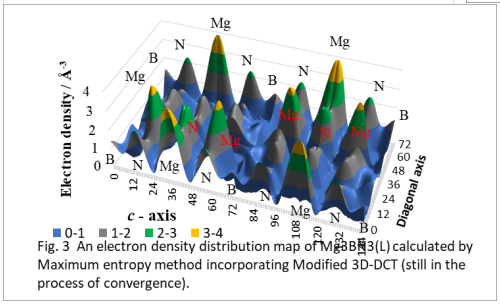

Fig. 3 An electron density distribution map of Mg_3BN_3(L) calculated by Maximum entropy method incorporating Modified 3D-DCT (still in the process of convergence).

1) H.Hiraguchi, The 104th CSJ Annual Meeting, H937-2pm-07, 2023. 2) H.HIRAGUCHI, O.SAKATA, H.HASHIZUME, A.TAKENAKA, O.FUKUNAGA.(1990). *J. Cryst. Soc.Jp.* OB-11, 32. 3) H. HIRAGUCHI, H. HASHIZUME, O. FUKUNAGA, A. TAKENAKA, M. SAKATA.(1991). *J. Appl. Cryst.* 24. 4) H. HIRAGUCHI, H. HASHIZUME, S. SASAKI, S. NAKANO, O. FUKUNAGA. (1993). *Acta Cryst.* B49. 5)H. HIRAGUCHI, (2021).*J.Appl.Cryst.* 6) M. Sakata & M. Sato, *Acta Cryst*. A46, 263-270, 1990. 7) M. Sakata, R. Mori, S. Kumazawa, M. Takata & H. Toraya, *J. Appl. Crvst.* 23, 526-534, 1990. 8) H.Hiraguchi, IUCr2023 in Melbourne.