Relationship Between Microwave Dielectric Properties and Chemical Bonding in R_2BaMO_5 (R=rare earth, M=Cu and Zn) Compounds

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The electric states of green phase-type R_2BaCuO_5 and R_2BaZnO_5 (R=rare earth) compounds were investigated by using the bond valence theorem and the first principle calculation method in order to clarify the relationship between the covalency of cation-oxygen bonds and microwave dielectric properties. By the R substitution for Y, the increase in the R-O distance in the R_2O_{11} polyhedron was recognized in both R_2BaCuO_5 and R_2BaZnO_5 compounds; this result took place the expansion of volume in the R_2O_{11} polyhedron. Moreover, the increase in the R-O distance of the R_2BaZnO_5 compound was recognized in comparison with that of R-O distance in the R_2BaCuO_5 compound because of the expansion of the bottom plane of MO_5 (M=Cu and Zn) pyramid caused by the Zn substitution for Cu. From the calculation of covalency of cation-oxygen bonds on the basis of bond valence theorem, it was shown that the covalency of R-O bond in the R_2BaCuO_5 and R_2BaZnO_5 compounds decreased with increasing the ionic radii of R ions. Comparing the covalency of R-O bond in the R_2BaZnO_5 compound with that of R_2BaCuO_5 compound, the covalency of R-O bond in R_2BaZnO_5 compound was smaller than that of R_2BaCuO_5 compound; this result is attributed to the differences in the R-O distances between the R_2BaCuO_5 and R_2BaZnO_5 compounds. The dielectric constant of both compounds was linearly increased from 14 to 18 with increasing the ionic radii of R ion, depending on the increase in the ionic polarizability of R ions. Then, the dielectric constant of R_2BaZnO_5 compound was large in comparison with that of R_2BaCuO_5 compound, though the ionic polarizability of Zn was smaller than that of Cu. Thus, it is considered that the difference in the dielectric constant between the R_2BaCuO_5 and R_2BaZnO_5 compounds is related with the covalency of R-O bonds.