Evaluation of Electronic State of $Mg_4(Nb_{2-x}Sb_x)O_9$ Microwave Dielectric Ceramics by First Principle Calculation Method

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The microwave dielectric ceramics with low dielectric loss are required for the microwave devices operated at high frequency; recently, the microwave dielectric properties of $Mg_4(Nb_{2-x}Ta_x)O_9$ solid solutions which have the corundum-type structure have been reported. As a result, it was found that the $Q\square f$ values of the solid solutions at x=2 are comparable to those of Al_2O_3 and the Ta substitution for Nb is effective in improving the $Q\square f$ values. However, the another element substitution for Nb in $Mg_4Nb_2O_9$ compound have not been clarified and the Sb^{5+} ion is considered to be the appropriate candidate as a substitution element for Nb because the Sb^{5+} ion has similar ionic radius to that of Nb^{5+} ion in the 6-coordinates.

Thus, the microwave dielectric properties of $Mg_4(Nb_{2-x}Sb_x)O_9$ solid solutions are evaluated and variations in the electric state of the solid solutions were investigated by using the first principle calculation method. The formation of single phase was observed from the X-ray powder diffraction patterns of the solid solutions sintered at 1400□ in the composition range of 0 to 1. The presence of MgO as a secondary phase was detected at the higher composition than x=1; this result is attributed to the vaporization of Sb in these compositions range. Comparing the overlap population of $(NbMg_{12}O_{45})^{-61}$ cluster model with that of $(SbMg_{12}O_{45})^{-61}$ cluster model, the slight covalent characteristic of Sb-O bond was recognized from the results of the first principle calculation method. In the composition range of 0 to 1, the $Q\square f$ values of $Mg_4(Nb_{2-x}Sb_x)O_9$ solid solutions sintered at 1400□ increased from 196000 to 280000 GHz; the dielectric constants of the solid solutions ranged from 13 to 10. However, the improvement in the temperature coefficient of resonant frequency by the Sb substitution for Nb was not recognized.