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Correlation between Structures and Microwave Dielectric Properties of $Ba_{3.75}Nd_{9.5-x}Sm_xTi_{17.5}(Cr_{1/2}Nb_{1/2})_{0.5}O_{54}$ Ceramics

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Abstract:

In this study, the influences of substitution of Sm^{3+} for Nd^{3+} on the crystal structure, Raman spectroscopy and microwave dielectric properties in $Ba_{3.75}Nd_{9.5}Ti_{17.5}(Cr_{1/2}Nb_{1/2})_{0.5}O_{54}$ (BNTCN) ceramics were investigated. The XRD results showed that all $Ba_{3.75}Nd_{9.5-x}Sm_xTi_{17.5}(Cr_{1/2}Nb_{1/2})_{0.5}O_{54}$ (BNTCN-S*x*) samples were crystallized as the orthorhombic tungsten-bronze type like structure. The unit cell volume of samples decreased as *x* increased, and the blue shift of Raman spectral peaks ($A_{g(1)}$ and B_g) also confirmed this result. Moreover, the increase of tilt angles indicated that more and more oxygen octahedra became more tilted, consequently leading to the decrease of temperature coefficient of resonant frequency (τ_f) with increase of *x* value. The packing fraction and $Q\times f$ value of BNTCN-S*x* ceramics reached the maximum value, whereas the FWHM of $A_{g(1)}$ and internal strain η reached the minimum value at $x = 3$. The low internal strain resulted from stability of the crystal structure, which was conducive to improvement of $Q\times f$ value in the BNTCN-S*x* ceramics. At last the BNTCN-S*x* ceramics sintered at 1380 ºC for 4h exhibited excellent microwave dielectric properties: $\varepsilon_r = 83.6$, $Q\times f = 11{,}597$ GHz, and $\tau_f = +1.3$ ppm/ºC when $x = 4$.

Key words: Rietveld analysis, Raman spectroscopy, Tilted oxygen octahedron, Microwave dielectric properties