Application of Nd (Mg½Ti ½) O3 (NMT) Perovskite in Mobile communications

Kouros Khamoushi, Mitic Vojislav, Jelena Manojlović, Vesna Paunović, *member of IEEE* and Goran Lazović

***Abstract* — The electrical conductivity, phase, and space group of property of the NMT substance and grain boundary of samples were approximated from complex compound by Raman spectroscopy, X-ray, SEM, TEM, and differential scanning calorimeter (DSC), samples prepared and analyzed in the laboratory in the frequency ranges from 9.76 GHz. The solid-state conventional method utilized. All the samples were tested by using XRD from 1250ºC to 1550ºC by increasing 50 degrees for every sample and cooling to the room temperature. The contraction of structure did not happen even at elevated temperature. The increase in Nd^+ ion polarizability is 0.50 nm compared to La^+ rare elements material, which is 0.60, this contributes to change of perovskite cubic. This is result of the smaller size of Nd^+ 0.127 nm cation compared to La^+ which increase number of dipoles despite the reduction of diploes and expands relative permittivity (ε_r). The single-phase material produced which shows quality factor $Q \times f$ = 60000 saturated at 10 GHz and temperature coefficient of (τ_f) = -77 MK^{-1}.** ***Keywords*: Microwave frequency; rare earth; electrical properties; quality factor; $Nd(Ln_{0.5}Ti_{0.5})O_3$ (Ln=Mg, Zn); Neodymium magnesium titanium oxide**.

1. Introduction

The tendency towards the highest level of homogeneous particle distribution in the entire volume of solids is their main propensity and characteristic. If the composition is closer to their desire arrangement, the phase transition is sharper and the structural order increases, which may explain the observed behavior, but this will not be convincing reason behind of the verification. It has long been believed in scientific circles that a large group of materials including ferroelectric oxides of complex structure from the perovskite or tungsten bronze family contain structural disturbances at crystallographic sites, which are result of diffuse phase transition (DPT).

The structure of our compound can be change using stoichiometric of other substances. Our desire is to achieve a great dielectric constant (ε_r), miniaturize the size of microwave which is in practical inversely related to dielectric constant $\varepsilon_r^{-1/2}$ and to receive a higher-level quality factor which indicates low tanδ and finer frequency tunability as well as superior filter. Because quality factor $Q = 1/\tan\delta$ also implies fine tunability and produce better filters. As a matter of fact, the compound of these ceramics has an important character in balancing of frequency flow because if the material naturally has lower heat property, then clearly it will be based on $\tau_f < 10\ MK^{-1}$. The high prevalence of perovskite material has brought great benefits in recent years due to their many excellent properties such as electrical properties in industrial and scientific applications. The advanced characterization of materials NMR, XPS, Neutron diffraction and Raman scattering studies are possible to influence leading information of semiconducting compound electronic, ionic property and dielectric materials [1-3].

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2. Experimental Procedure

The lab work for preparation of sample is depicted in detail in references [4]and [5]. Here is a short sketch of the method.

The following pure powders (99.98% 99.99%) used for preparation of samples: Nd_2O_3, TiO_2, ZnO, and $(MgCo_3)_4Mg(OH)_25H_2O$. Powder of the rare-earth oxide was mixed with water for fourteen hours and ball mill with agent to form Hexagonal $Nd(OH)_3$. The stoichiometric volume of powder was mixed in mill with water around four hours.

Then, powders were mixed with deflocculant and finally mixture was dried around eighty centigrade degrees just about twelve hours. The fine particles were filtered and hard-pressed applying 1275 kg/ cm^2, the area of pellets was A=11 cm^2. Sintering occurred for six hours from 1250°C to 1550°C. Pellets were weigh up using Archimedes' method before and after sintering to compute the degree of deficiency. Dense and homogeneous ceramic powder of neodymium magnesium titanium oxide was obtained after pressing powder using 1275 kg/ cm^2 pressure and sintering at 1550°C for around six hours.

To ensure the microstructure and surface analyses of the samples as well as definition of phase group XRD and SEM were used. The quality factor and relative permittivity were measurement at frequency of microwave by a standard method of Hakki and Coleman [6]. The electrical measurement of $Q \times$f, and τ_f were measured using (HP-8719 C 50 MHz -13.5 GHz) device.

To measure quality factor a cylindrical resonance cavity was used. A cavity was made of a superior metal with higher conductivity which had 4 times larger size than sample and it located in inner part with a support which did not affect the property of sample. The coupling loop were connected to a computer and monitor to measure loaded quality factor.

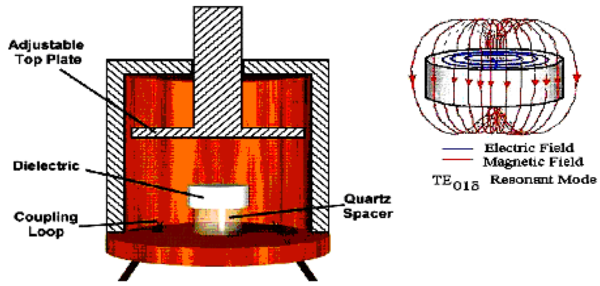

Fig.1. The device for measuring electrical property of sample [7].

Figure 2. shows the schematic resonance peak for definition of loaded quality factor (Q_L) which was determined experimentally from the shape of resonance peak. A peak will be generated during the transmission signal and its amplitude will be equal to resonance frequency. The peak has a finite width, and its band width (BW) will be defined as the width of peak at half of its Maximum value. It is 3 dB from the peak.

The quality factor measured using following formula:

$Q_0 = (f_0 / \Delta f) / (1-10^{-(IL/20)})$

$TE_{01\delta}$ = resonant mode

f_0 = resonant frequency

Δf = 3 dB bandwidth

IL = Insertion loss

Prior to test, powder sample was pressed into pellet using 1275 kg/cm^2 with surface area equal to 11 cm^2.

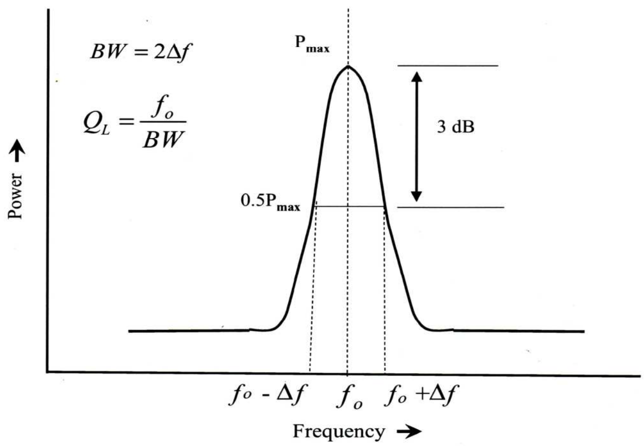

Fig.2. Schematic resonance peak illustrates the definition of Loaded quality factor Q_L [7].

3. Results and Discussion.

Figure 3 demonstrates the measurement of sintering versus density for neodymium zinc titanium oxide (NMT). As the heat raises the density of NMT increased and reached (94% ρ_{th}) at 1500°C, then it increased to (98% ρ_{th}) at 1550°C, which indicates high quality and totally dense material. Theoretical density measurement is illustrated and indicates the amount of porosity in our material, it defines if material is dense or there is vacancy or porosity. This is vital specially in the case of Oxide perovskite.

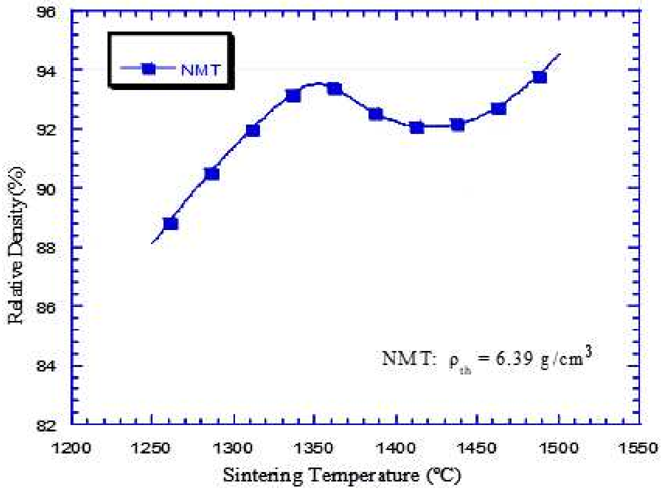

Fig. 3. NMT samples after sintering for six hours at 1250-1550 ºC [7].

XRD patterns of NMT samples sintered at 1675ºC temperature. For comparison NMT PDF card number 77-2426 were used. all the samples' peaks match PDF card number 77-2426. Crystallography indicates that crystal monoclinic structure can be purposed for that with lattice parameter equal to a= 55 nm, b = 56 nm c = 0.78 nm, angle of a = 90º, γ = 90º, β = 89.01º (Figure 4).

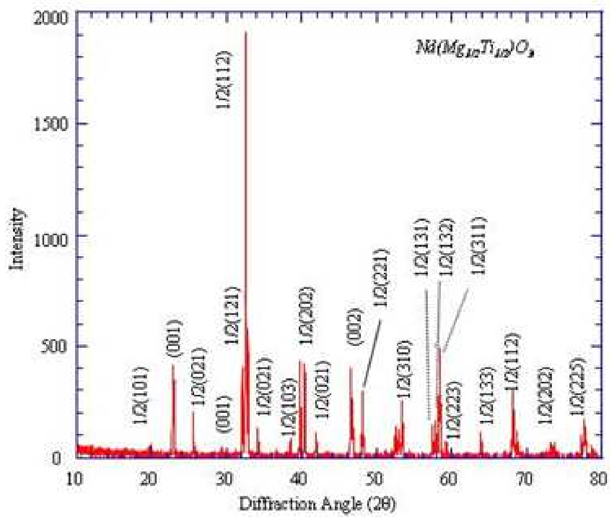

Fig. 4. XRD measurement for samples of NMT sintered around 1675ºC about four hours.

SEM secondary electron images of $Nd(Mg_{1/2}Ti_{1/2})O_3$ illustrated in Figure 5. Images are demonstrating sintering temperature of NMT at 1650°C. The grain size is around one to five micrometers in average. It illustrated a dense ceramic which has a single phase. Sample also shows only one homogeneous color, and this is one of the tests to define single-phase material. If the sample exhibit two different colors in contrast, then material is not single-phase, probably there is impurity, or another phase is present in the sample. However, several samples of NMT tested and all the result shows a pure and extremely dense NMT material.

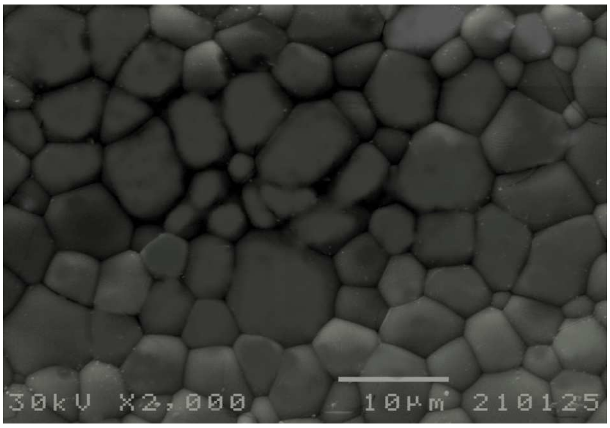

Fig.5. Sample of NMT beam sintered at 1650 °C, shows a dense and single-phase material. The beam is in [111] direction.

3.1. NMT Microstructure

The XRD arrangement of sample powder (NMT) demonstrated in Figure six, it is well matched with research work of D.Y.Lee *et al.* [8] and M.P Seabra *et al.* [9] and recent research of Vojislav V. Mitic *et al.* [10].

To index the NMT for assessment the sample was compared to standard PDF card number 77-2426 with lattice parameter of a= 55 nm, b = 56 nm c = 0.78 nm, monoclinic formation as well as single-phase material. Experimental samples tested by XRD are identical to the standard one and there were not any differences between them. In fact, there was an excellent similarity between both calcined and sintered samples. Still, for further research, the group are planning to perform Density Functional Theory (DFT) which is a quantum mechanics computational investigation of the electronic structure of material mainly at the ground state of many-body systems, to define atoms, molecules, and the phases in the material and finally, to be able to suggest an atomic and 3-dimensional model for the perovskite sample and as well as to propose a space group for crystal structure of sample.

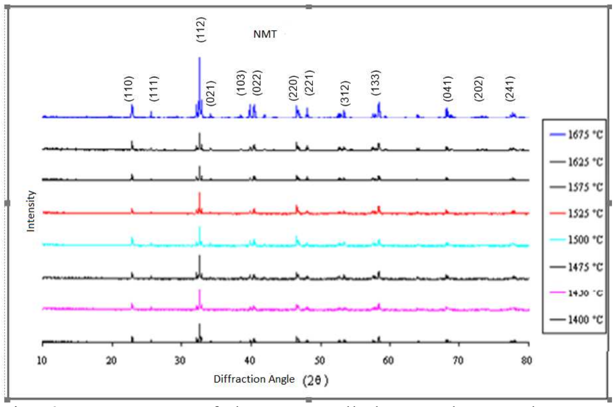

Fig. 6. XRD pattern of the NMT. All the samples are shown a regular structure.

4. Conclusions and Future Work

The systematic research work of NMT dielectric material considered to estimate the dielectric properties and space group of NMT. The research and result of calculation show that NMT has lattice parameter of a = 55 nm, b = 56 nm c = 0.78 nm**,** it shows a monoclinic crystal structure. The theoretical density is 6.0846 g/cm^3 and τ_f = -77 MK^{-1} for NMT. The quality factor for NMT was 60000 to be saturated at frequency 9.76 GHz. The dielectric constant of NMT is equal to 25. The research of this investigation demonstrates the NMT materials express a great ability for wireless communication.

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