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Original Article

Structure, bond characteristics and microwave dielectric properties of new $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ (A=Ni, Co, Zn and Mg) ceramics based on complex chemical bond theory

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ABSTRACT

Tri-rutile structured $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ (A=Ni, Co, Mg, Zn) ceramics were synthesized using traditional solid reaction method. The crystal structures were studied by X-ray diffraction in conjunction with Rietveld refinement analysis. Based on the complex chemical bond theory and crystallographic data, some principle chemical bond characteristics such as bond ionicity, lattice energy, bond energy and coefficient of thermal expansion of complex $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ ceramics were obtained through quantitative calculation. The calculated results provided useful information to clarify the correlations between chemical bond characteristics and microwave dielectric properties of $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ ceramics. The dielectric constant was closely associated with the ionicity of Ta−O bond, and the $Q \times f$ values were correlated with the lattice energy of Ta−O bond. The τ_f values were affected by the bond energy of Ta−O bond and the coefficient of thermal expansion of A−O bond.

1. Introduction

Microwave dielectric materials with medium dielectric constant (ε_r) and high-quality factor (Q) have become more important in recent years as the rapid development of mobile phone and wireless communication market [1]. Compared with various microwave dielectric materials with medium dielectric constant, $ATiNb_2O_8$ (A = Zn, Mg, Ni, Co et al.) ceramics exhibit excellent properties [2–7]. Considering that Ta^{5+}(0.64 Å) has similar ionic radii to that of Nb^{5+}(0.64 Å) [8], it is possible to prepare the $ATiTa_2O_8$ microwave dielectric ceramics similarly as the $ATiNb_2O_8$. For example, the new tri-rutile type structured ceramics $Co_{0.5}Ti_{0.5}TaO_4$ with excellent microwave properties of $\varepsilon_r = 40.69$, $Q \times f = 17{,}291$ GHz and $\tau_f = 114.54$ ppm/°C, were reported by Hongyu Yang et al., and the correlations between crystal structure and microwave properties were explained based on the P-V-L theory, Clausius-Mossotti relationship and oxygen distortions of the octahedron [9]. However, to our knowledge, there was no specific research on the correlations between bond characteristics and microwave dielectric properties of the $ATiTa_2O_8$ microwave dielectric ceramics. As we know, the complex chemical bond theory, usually applied to complex crystals calculations, can explain many basic properties of crystals in some extent. It has been widely used in analyzing the effects of intrinsic factors such as bond ionicity, lattice energy and bond energy on the properties of microwave dielectric ceramics [10–16]. Therefore, in this study, the $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ (A=Ni, Co, Zn and Mg) ceramics were prepared via traditional solid reaction method, and the correlations between chemical bond characteristics (such as bond ionicity, lattice energy, bond energy and coefficient of thermal expansion) and microwave dielectric properties were investigated for the first time.

2. Experimental procedure

All samples were prepared via traditional solid reaction method. High - purity NiO (99.9), CoO(99.9), ZnO(99.9), MgO(99.9) TiO_2 (99.99), Ta_2O_5 (99.99) powders were adopted as raw materials. Firstly, the stoichiometric powder mixtures were ball milled for 4 h using alcohol as milling medium. Further, the slurry was quickly dried at the temperature of 70 °C and sieved through 200 mesh. Secondly, after presintered at the temperature range of 1100 °C–1250 °C for 2 h, the powders were ball-milled, dried and sieved again. Then with 5 wt% polyvinyl alcohol (PVA) added as the blinder, the synthetic powders were pressed into pellets under the pressure of 200 MPa. Finally, the green pellets were sintered at 1150 °C–1350 °C for 4 h with a heating rate of 5 °C /min.

X-ray diffractometer (XRD, Rigaku, DMAX-RB, Japan) with Cu Kα radiation, scanning from 10° to 90° with a step of 0.02°, was employed to analyze the crystal structure of ceramics. The crystallographic parameters were acquired from the Rietveld refinement of the XRD data

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using GSAS-EXPGUI software [17,18]. Parameters including background, scale factor, lattice parameters, atomic coordinates, isotropic thermal parameters and profile parameters (U, V, W and shift) were refined step by step until the final results were reliable (Rwp < 10 %). The microstructure of the ceramics was observed using a scanning electron microscopy (SEM, JSM-6710 F, JEOL, Japan). The density of ceramics was confirmed by a method based on Archimedes principle. Microwave dielectric properties of the ceramics were measured by a network analyzer (8720ES, Agilent, USA) using Hakki-Coleman's dielectric resonator method [19–21]. All measurements were conducted at the frequency of 6–9 GHz. The temperature coefficients of the resonant frequency (τ_f) were measured over the range of temperature from 20 to 80 °C. The τ_f values were calculated in accordance with the following formula:

$$\tau f = \frac{f_2 - f_1}{f_1(T_2 - T_1)} \tag{1}$$

where f_1 and f_2 are the resonant frequency at T_1 and T_2.

3. Result and discussion

Fig. 1 shows the XRD patterns of $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ (A=Ni, Co, Zn and Mg) ceramics sintered at optimum temperature for 4 h. All diffraction peaks for each compound well matched tri-rutile structure (JCPDS: #32-0702) with $P4_2/mnm$ space group, and no other second phase was indexed. Based on the results of XRD patterns, Rietveld refinement by GSAS-EXPGUI was performed on these compounds. The XRD profile of $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ ceramics after refinement are shown in Fig. S1 (see the Supplementary Information (SI)). The calculated patterns of all samples closely fitted those of measured, which indicated that the refinement results were credible. In addition, the crystallographic data of these four ceramics are also summarized in Table 1. Due to the different types of A-site ions, there lied slight change in the unit cell volume of these four ceramics.

To further study the crystal structure of these four ceramics in detail, refined atomic fractional coordinates of $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ ceramics are given in Table S1 (SI). In the crystal structure of $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$, the cations occupied the 2a and 4e Wyckoff positions, while 4f and 8 j Wyckoff positions were distributed by all O anions. Fig. 2 shows the crystal structure diagram of these four ceramics. All cations were connected with six O anions to form [M1O_6] and [M2O_6] octahedron. [M1O_6] was surrounded by [M2O_6] octahedron and connected to [M2O_6] by sharing common-edged (such as O1-O1). Moreover, the interatomic distances (Å) of $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ ceramics are listed in Table S2 (SI). It could be noticed that the M2—O2 bond showed two

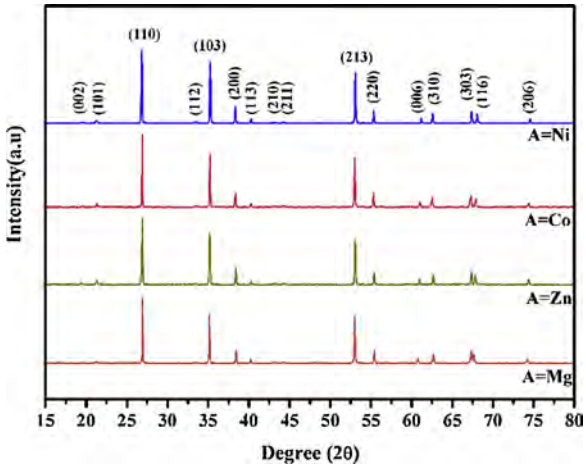

Fig. 1. The XRD patterns of $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ (A=Ni, Co, Zn and Mg) ceramics sintered at optimum temperature for 4 h.

different bond length. Owing to the different bond length, the distortion degree of octahedron was quite distinct (see Fig. 2).

Fig. 3 shows the SEM images of $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ ceramics sintered at optimum temperature for 4 h. Compact microstructure observed from Fig. 3 demonstrated that all samples were sintered properly. Furthermore, the densities and microwave dielectric properties of $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ ceramics are listed in Table 2. It could be seen that all samples possessed the relative density more than 94 %, medium dielectric constants, high $Q \times f$ values and small τ_f values.

In order to clarify the correlations between the crystal structure and microwave dielectric properties of $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ ceramics, the complex chemical bond theory was carried out. Combined with crystallographic data and the complex chemical bond theory, the complex $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ compounds could be decomposed into the sum of binary crystals [22]. As a representative, the binary expression of $Ni_{0.75}Ti_{0.75}Ta_{1.5}O_6$ compound after decomposition was shown in Eq. (2) (others see the Eqs. (S1)–(S3) (SI)):

$$\begin{aligned} Ni_{0.75}Ti_{0.75}Ta_{1.5}O_6 = {} & Ni_{1/4}O^1{}_{1/2} + Ni_{1/2}O^2{}_1 + Ti_{1/4}O^1{}_{1/2} + Ti_{1/2}O^2{}_1 \\ & + Ta^1{}_{1/12}O^1{}_{1/6} + Ta^1{}_{1/6}O^2{}_{1/3} + Ta^2{}_{5/12}O^1{}_{5/6} \\ & + Ta^2{}_{10/12}O^2{}_{5/3} \end{aligned} \tag{2}$$

According to the binary expressions, there were three kinds of chemical bonds in each crystal, namely A—O (AN=i, Co, Zn and Mg), Ti—O and TaO— bonds. The effective valence electron number of cations were $Z_A = 2$, $Z_{Ti} = 4$ and $Z_{Ta} = 5$, respectively, while that of O anions were $Z_O = 3$ in A—O bond, $Z_O = 6$ in Ti—O bond and $Z_O = 15/2$ in Ta—O bond, respectively. In addition, the coordination number and charge distribution of ions are depicted in Fig. S2 (SI).

Generally, there is a close relationship between the dielectric constant and bond ionicity [14]. Based on the complex bond theory, the bond ionicity (f_i^μ) of each chemical bond μ were calculated as the following equation [10]:

$$f_i^\mu = \frac{(C^\mu)^2}{(E_g^\mu)^2} \tag{3}$$

Where E_g^μ is the average energy gap for the bond μ, and C^μ is the heteropolar part of E_g^μ (more information of E_g^μ and C^μ see Eqs. (S4)–(S7) (SI)). The calculated results are listed in Tables S3–S6 (SI), and the average bond ionicity of A—O, Ti—O and Ta—O bonds are depicted in Fig. S3 (SI, green bars). It was observed that the $f_{i(Ta-O)}$ was the strongest, followed by $f_{i(Ti-O)}$ and $f_{i(A-O)}$ in each ceramic. The relationship between $f_{i(Ta-O)}$ and dielectric constant is revealed in Fig. 4. Overall, the variation of dielectric constant showed positive correlation with $f_{i(Ta-O)}$. The dielectric constant which changed with chemical bond ionicity was mainly due to the different interaction between anions and cations [10,14]. Based on the results, it could be concluded that $f_{i(Ta-O)}$ played a key role in the dielectric constant of $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ ceramics.

Lattice vibration in crystals is a major factor affecting $Q \times f$ values of microwave dielectric ceramics. Zhang et al. proposed a method to calculate the lattice energy (U) using the chemical bond properties, shown as Eq. (4) [23]:

$$U_{cal} = \sum_\mu U_{bc}^\mu + U_{bi}^\mu \tag{4}$$

Where U_{bi} is the ionic part and U_{bc} is the covalent part of μ bond (more information of E_g^μ and C^μ see in Eqs. (S8)–(S9) (SI)). The calculated results are given in Tables S3–S6 (SI), and Fig. S3 (SI, pink bars) shows the average lattice energy of A—O, Ti—O and Ta—O bonds. Obviously, Obviously, there was the sequence of $U_{Ta-O} > U_{Ti-O} > U_{A-O}$, which meant that U_{Ta-O} made the predominant contribution to the total lattice energy. Fig. 5 shows the relationship between $Q \times f$ values and U_{Ta-O}. It was found that the $Q \times f$ values shared the similar tendency with U_{Ta-O}. Generally, a crystal with higher lattice energy implied its weaker lattice vibration, thus leading to a lower intrinsic loss and a higher $Q \times f$ value

Table 1
Crystallographic data obtained from Rietveld refinement for $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ (A=Ni, Co, Zn and Mg) ceramics.

Chemical Composition	Scpace group	lattice Parameters(Å)			V_{unit}(Å^3)	Reliability factors		
		a = b(Å)	c(Å)	α = β = γ		Rwp (%)	Rp (%)	χ^2
$Ni_{0.75}Ti_{0.75}Ta_{1.5}O_6$	P42/mnm	4.6869(2)	9.0726(1)	90	199.30(0)	9.84	7.32	1.36
$Co_{0.75}Ti_{0.75}Ta_{1.5}O_6$	P42/mnm	4.7030(4)	9.1207(3)	90	201.78(3)	8.82	6.04	3.82
$Zn_{0.75}Ti_{0.75}Ta_{1.5}O_6$	P42/mnm	4.6980(0)	9.0963(0)	90	200.76(7)	9.33	6.69	1.42
$Mg_{0.75}Ti_{0.75}Ta_{1.5}O_6$	P42/mnm	4.6897(6)	9.1467(3)	90	201.17(2)	7.82	5.78	3.13

[24–26]. In conclusion, U_{Ta-O} could be considered as a predominant intrinsic factor affecting the $Q \times f$ values of $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$(A=Ni, Co, Mg, Zn) ceramics.

The bond energy (E) and coefficient of thermal expansion (α) of a complex crystal could be acquired by the following Eqs [10]:

$$E = \sum_{\mu} \left[\frac{(r_{cA} + r_{cB})}{d_{\mu}} (E_{A-A} E_{B-B})^{1/2} t_c + \frac{33200}{d^{\mu}} t_i \right] \quad (5)$$

$$\alpha = \sum_{\mu} (-3.1685 + 0.8376\gamma_{mn}) F^{\mu}_{mn} \quad (6)$$

Where t_c and t_i are covalent and ionic coefficients of chemical bonds, respectively. r_{cA} and r_{cB} are the covalent radii. d_{μ} is the bond length. $E_{A\text{-}A}$ and $E_{B\text{-}B}$ are the bond energy [27]. F^{μ}_{mn} is the proportion of μ bond in the total bonds of a supercell and γ_{mn} is a parameter obtained from the ref [10]. The calculated results are listed in Tables S3–S6 (SI). The average bond energy and the coefficient of thermal expansion of A—O, Ti—O and Ta—O bonds are illustrated in Fig. S3 (SI, blue bars and pink bars, respectively). As shown in Fig. S3, Ta—O bond had the highest bond energy while A—O bond had the largest thermal expansion coefficient. Fig. 6 exhibits the relationship among E_{Ta-O}, α_{A-O} and τ_f values. Apparently, the varying tendency of α_{A-O} was the same as τ_f values, whereas E_{Ta-O} showed opposite trend with τ_f values. It was well known that a crystal with higher bond energy and lower coefficient of thermal expansion indicated better thermal stability. Therefore, in this work, both E_{Ta-O} and α_{A-O} were regarded as key factors affecting the τ_f values of $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ ceramics.

4. Conclusions

The correlations between chemical bond characteristics and microwave dielectric properties of $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$(A=Ni, Co, Mg, Zn) ceramics prepared via traditional solid reaction method were investigated. All $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ ceramics maintained a tri-rutile structure and exhibited medium dielectric constant of 39.01–43.35, high $Q \times f$ values of 18,320–25,051 GHz and τ_f values of 75–87.6 ppm/°C. Based on the calculated results, the Ta—O bond possessed the strongest bond ionicity, the highest lattice energy and bond energy, while the A—O bond had the largest coefficient of thermal expansion. The dielectric constant was closely associated with the ionicity of Ta—O bond. The $Q \times f$ values were dependent on the lattice energy of Ta—O bond. The τ_f values were affected by the bond energy of Ta—O bond and the coefficient of thermal expansion of A—O bond. The analysis results could lay a theoretical foundation for the future research of $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ ceramics.

We declare that we have no financial and personal relationships with other people or organizations that can inappropriately influence our work, there is no professional or other personal interest of any nature or kind in any product, service and/or company that could be construed as influencing the position presented in, or the review of, the manuscript entitled, “Structure, Bond Characteristics and Microwave Dielectric Properties of New A0.75Ti0.75Ta1.5O6 (A=Ni, Co, Zn and Mg) ceramics Based on Complex Chemical Bond Theory”.

Declaration of Competing Interest

We declare that we have no financial and personal relationships with other people or organizations that can inappropriately influence

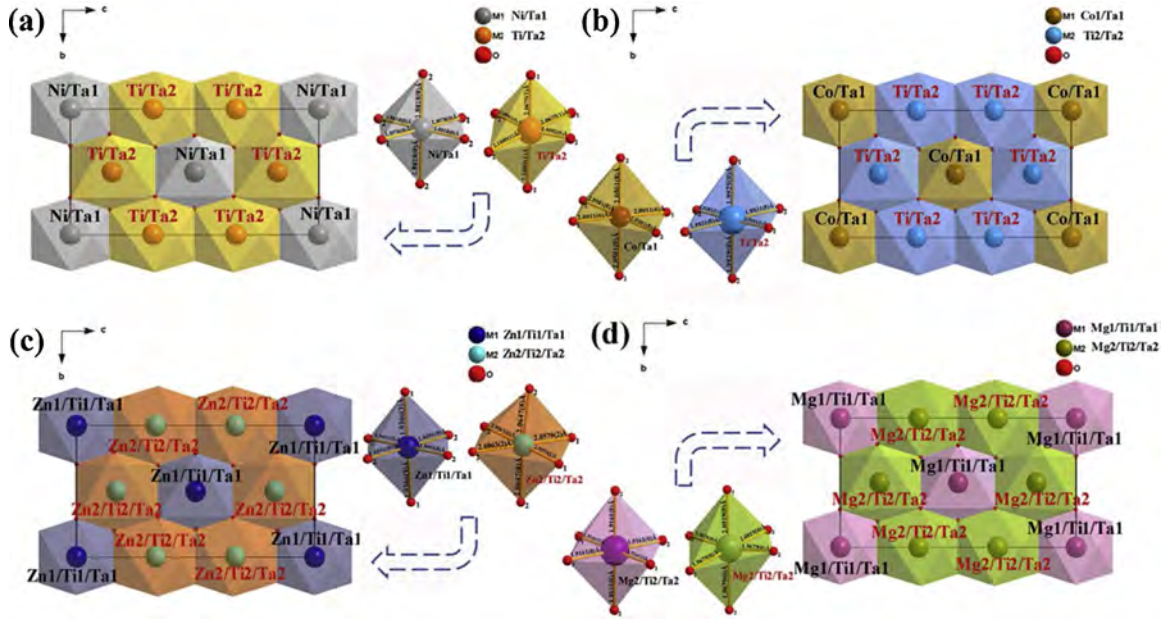

Fig. 2. The schematic diagram of the crystal structure of **a** $Ni_{0.75}Ti_{0.75}Ta_{1.5}O_6$, **b** $Co_{0.75}Ti_{0.75}Ta_{1.5}O_6$, **c** $Zn_{0.75}Ti_{0.75}Ta_{1.5}O_6$, **d** $Mg_{0.75}Ti_{0.75}Ta_{1.5}O_6$ ceramics.

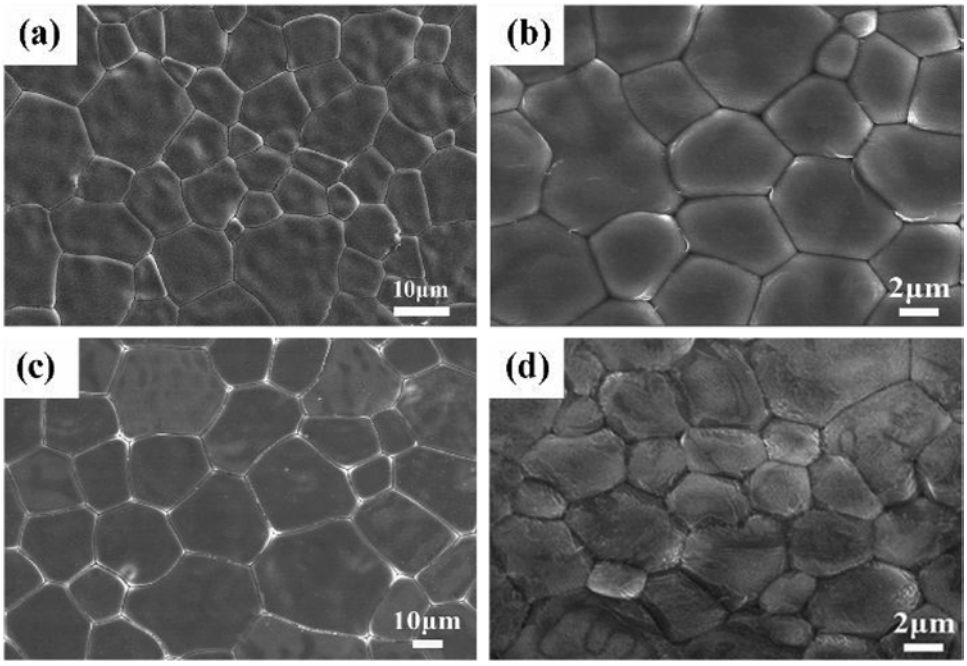

Fig. 3. SEM images of **a** $Ni_{0.75}Ti_{0.75}Ta_{1.5}O_6$, **b** $Co_{0.75}Ti_{0.75}Ta_{1.5}O_6$, **c** $Zn_{0.75}Ti_{0.75}Ta_{1.5}O_6$, **d** $Mg_{0.75}Ti_{0.75}Ta_{1.5}O_6$ ceramics sintered at optimum temperature for 4 h.

Table 2
Sintering temperature, density and microwave properties of $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ (A=Ni, Co, Zn and Mg) ceramics (Mean ± SD).

Chemical Composition	St (°C)	Buck Density (g/cm^3)	Relative Density (%)	ε_r	$Q \times f$ (GHz)	τ_f (ppm/°C)
$Ni_{0.75}Ti_{0.75}Ta_{1.5}O_6$	1350	7.0155 ± 0.02	94.70 ± 0.30	39.86 ± 0.22	25051 ± 300	75 ± 0.84
$Co_{0.75}Ti_{0.75}Ta_{1.5}O_6$	1150	7.0443 ± 0.03	95.71 ± 0.33	39.01 ± 0.26	16796 ± 124	77.97 ± 0.92
$Zn_{0.75}Ti_{0.75}Ta_{1.5}O_6$	1250	7.1815 ± 0.05	96.01 ± 0.43	43.35 ± 0.18	19852 ± 331	77.1 ± 0.73
$Mg_{0.75}Ti_{0.75}Ta_{1.5}O_6$	1350	6.6442 ± 0.03	95.51 ± 0.29	42.83 ± 0.03	18320 ± 292	87.6 ± 0.51

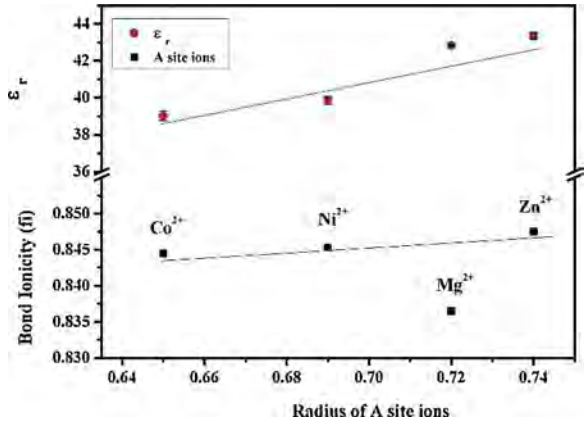

Fig. 4. Bond ionicity ($f_{i(Ta-O)}$) and dielectric constants as a function of radius of A site cations in $A_{0.75}Ti_{0.75}Ta_{1.5}O_6$ ceramics.

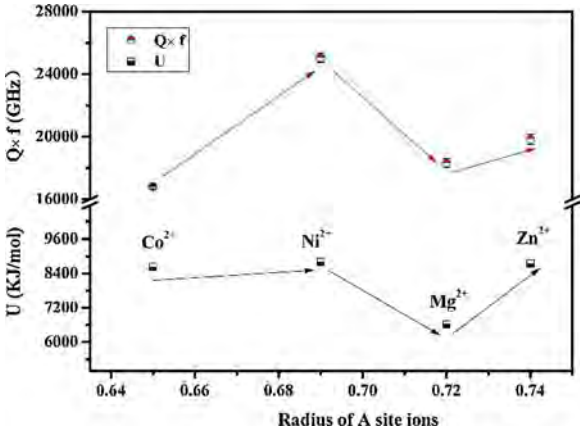

Fig. 5. $Q \times f$ values and lattice energy (U_{Ta-O}) as a function of radius of A site cations.

our work, there is no professional or other personal interest of any nature or kind in any product, service and/or company that could be construed as influencing the position presented in, or the review of, the manuscript entitled, “Structure, Bond Characteristics and Microwave Dielectric Properties of New A0.75Ti0.75Ta1.5O6 (A=Ni, Co, Zn and Mg) ceramics Based on Complex Chemical Bond Theory”.

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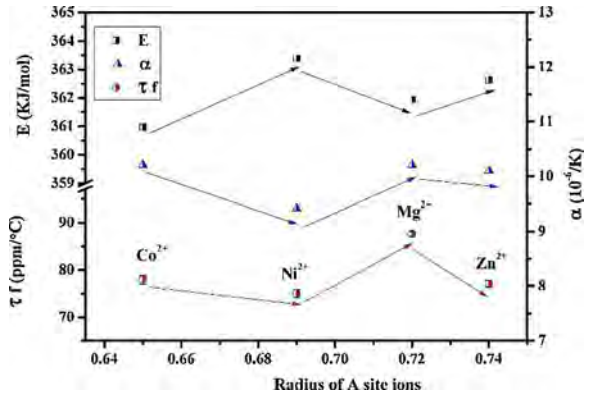

Fig. 6. The bond energy (E_{Ta-O}), the coefficient of thermal expansion (α_{A-O}) and τ_f values as a function of radius of A site cations.

Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:https://doi.org/10.1016/j.jeurceramsoc.2019.11.086.

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