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Feature article

A novel formula for the quality factor calculation for the multiphase microwave dielectric ceramic mixtures

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ABSTRACT

Microwave dielectric ceramics are pillar materials in the microwave applications, for example, resonators. However, because most ceramics possess non-zero temperature coefficients, two or more ceramics, with temperature coefficient of opposite signs, are always mixed as a multiple phase system to obtain a zero temperature coefficient ceramic. While the dielectric constant can be calculated by the Maxwell-Wagner based formula, the quality factor (Q) is usually hard to be precisely calculated by the conventional method. In this paper, basing on the classical dispersion theory, we derive a new formula for the Q calculation for the ceramic mixtures. The deviation between the calculated and reported Q, of several typical ceramic systems, is around ±5%, for the example of two phases ceramic mixtures.

1. Introduction

Microwave dielectric ceramics have been widely utilized in microwave applications, for example, resonators, because of their high dielectric constant (ε_r) and high quality factor (Q) [1–6]. Dielectric constant of ε_r can result in the size of devices being $\varepsilon_r{}^{1/2}$ times smaller; high quality factor (Q), which is approximately the reciprocal of the dielectric loss ($tan\delta$), represents low energy loss and precise frequency selection [1,2,4].

In practice, ceramics are always needed to be mixed to form multiphase mixtures to stabilize the work frequency, in other words, to obtain a ceramic with a zero temperature coefficient at the resonant frequency [2,7–13]. While the composites' dielectric constant can be well predicted by the Maxwell-Wagner formula, the issue of the quality factor calculation has not been well solved yet [3,14–16]. Traditionally, the quality factor (Q) is estimated by:

$$Q^{-1} = \sum_{i=1}^{n} V_i Q_i^{-1}, \tag{1}$$

in which n corresponds to the number of ceramics to be mixed, V_i is the volume molar ratio of the i-th ceramic, $\sum_{i=1}^{n} V_i = 1$, and Q_i is the quality factor of the i-th ceramic [15,17]. The equation only considers all starting materials' Q, and it shows a simple superposition relationship. The actually reported results show other kinds of variation curves [15,16]. The deviation between the Eq. (1) calculated and actually measured results is large, for example, in Refs. [15] and [16].

In this paper, based on the definition of dielectric loss in the classical dispersion theory, we will derive the total dielectric loss (Q^{-1}) of the multiphase ceramic mixtures. After that, we apply the formula to calculate the quality factor of ceramic mixtures and compare them to the reported results. Relative deviation also will be given to confirm the effectiveness of the new formula.

2. Theory

In the classical dispersion theory, the complex dielectric constant of one ceramic is in the form of:

$$\varepsilon = \varepsilon' + i\varepsilon'', \tag{2}$$

in which,

$$\varepsilon' = \varepsilon_\infty + \sum_j 4\pi\rho_j \upsilon_j^2 \frac{\upsilon_j^2 - \upsilon^2}{\left(\upsilon_j^2 - \upsilon^2\right)^2 + \gamma_j^2 \upsilon^2}, \tag{3}$$

$$\varepsilon'' = \sum_j 4\pi\rho_j \upsilon_j^2 \frac{\gamma_j \upsilon}{\left(\upsilon_j^2 - \upsilon^2\right)^2 + \gamma_j^2 \upsilon^2}, \tag{4}$$

where ε_∞ is the permittivity caused by electronic polarization, $4\pi r_j$ is the strength of the oscillator, γ_j is phonon damping factor, ν_j is the phonon eigen frequency and ν is the measured microwave frequency ($\nu << \nu_j$, so $\nu_j - \nu \approx \nu_j$), and $i^2 = -1$ [1]. The dielectric loss of the ceramic is defined as [1]:

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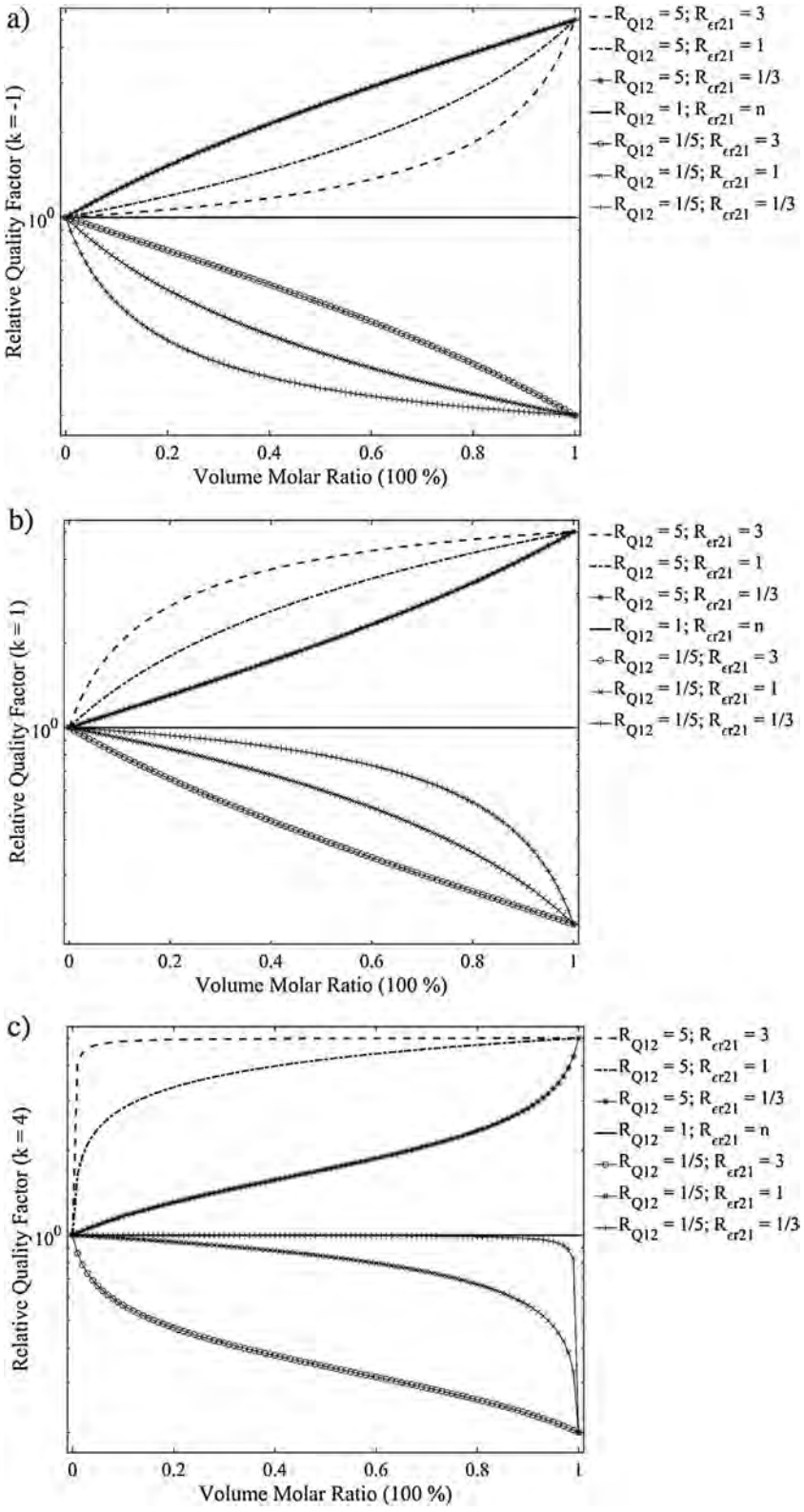

Fig. 1. The relative quality factor versus dielectric constant ratio, dielectric loss ratio and volume molar ratio: (a). $k = -1$; (b). $k = 1$ and (c). $k = 4$.

$$\tan\,\delta = \frac{\varepsilon''}{\varepsilon'} \approx \frac{\upsilon \sum_j \frac{4\pi\rho_j\gamma_j}{\upsilon_j^2}}{\varepsilon_\infty + \sum_j 4\pi\rho_j}. \tag{5}$$

Similarly, when mixing two or more ceramics as a multiphase material system, we assume that the total dielectric loss shows the same format as Eq. (5), determined by the ratio between the total imaginary and the total real parts of the dielectric constant of the mixture. In the following, we will write the i-th real part of the complex dielectric constant, ε_i' as dielectric constant ε_{ri} for sim-

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plicity. The real part of the dielectric constant of the mixture could be predicted by the Maxwell-Wagner formula [14,15]:

$$\varepsilon_r = \left(\sum_{i=1}^{n} V_i \varepsilon_{ri}^k\right)^{1/k} \tag{6}$$

where ε_{ri} is the dielectric constant of the i-th ceramic, and k can be determined by the experimental results. In the experimental part, we will show how to obtain the k value of a mixture. From Eq. (5), [1] claims that the $tan\delta$ is linearly frequency dependent for a ceramic and the claim has been widely accepted [1]. In other words, the imaginary part of the dielectric constant of the multiphase ceramics also obey Eq. (6). Therefore, the dielectric loss of the mixture can be obtained from Eqs. (5) and (6). After some algebra steps, we can get the total dielectric loss:

$$\tan^k\delta = \frac{\sum_{i=1}^{n} V_i \varepsilon_{ri}^k \tan^k\delta_i}{\sum_{i=1}^{n} V_i \varepsilon_{ri}^k} \tag{7}$$

in which $tan\delta_i$ is the dielectric loss of the i-th ceramic. In practice, people would like to use quality factor,

$$Q^{-1} = tan\delta \tag{8}$$

in which Q is the quality factor of a ceramic. So we write Eq. (7) in terms of Q:

$$Q^{-k} = \frac{\sum_{i=1}^{n} V_i Q_i^{-k} \varepsilon_{ri}^k}{\sum_{i=1}^{n} V_i \varepsilon_{ri}^k}. \tag{9}$$

In this equation, the quality factor of the mixture (Q) actually depends not only on the quality factor (Q_i) of each ceramic, but also the dielectric constant, ε_{ri}, and how it varies, k. Until now, basing on the above equations, quality factor of a multiphase ceramic can be calculated. In the following, we write Eq. (9) in a different form, for clear data comparison.

Usually, the target is to modify the properties of the first material, whose quality factor and dielectric constant are Q_1 and ε_{r1}, so we rewrite Eq. (9):

$$\left(\frac{Q_1}{Q}\right)^k = \frac{\sum_{i=1}^{n} V_i \left(\frac{Q_1}{Q_i}\right)^k \left(\frac{\varepsilon_{ri}}{\varepsilon_{r1}}\right)^k}{\sum_{i=1}^{n} V_i \left(\frac{\varepsilon_{ri}}{\varepsilon_{r1}}\right)^k} \tag{10}$$

If we define the relative quality factor R_Q, R_{Q1i}, and relative dielectric constant ratio $R\varepsilon_{ri1}$ as following:

$$R_Q = \frac{Q_1}{Q}; \tag{11}$$

$$R_{Q1i} = \frac{Q_1}{Q_i}; \tag{12}$$

$$R_{\varepsilon_r i1} = \frac{\varepsilon_{ri}}{\varepsilon_{r1}}. \tag{13}$$

Then we can obtain the following equation:

$$R_Q^k = \frac{\sum_{i=1}^{n} V_i R_{Q1i}^k R_{\varepsilon_r i1}^k}{\sum_{i=1}^{n} V_i R_{\varepsilon_r i1}^k}. \tag{14}$$

In other words, once parameters in Eqs. (12)–(13) and k are determined, the quality factor of the multiphase mixture could be calculated. In practice, most reports are actually mixing two ceramics to form multiphase ceramics [7–13]. Even more than two ceramics mixing can be calculated by the same rule. Thus we in the following will give several examples of two-phase-ceramic systems, in the form of (1-V) A – V B. Then, with the dielectric constant and quality factor of these two ceramics, Eq. (14) could be written as:

$$(R_Q)^k = \frac{1 - V + R_{\varepsilon_{r21}}^k R_{Q12}^k V}{1 - V + R_{\varepsilon_{r21}}^k V}. \tag{15}$$

As discussed above, the quality factor is determined by parameters, V, R_{Q12}, $R\varepsilon_{r21}$ and k. The k value could be negative and positive, small and large. For a given mixing system, there is only one k.

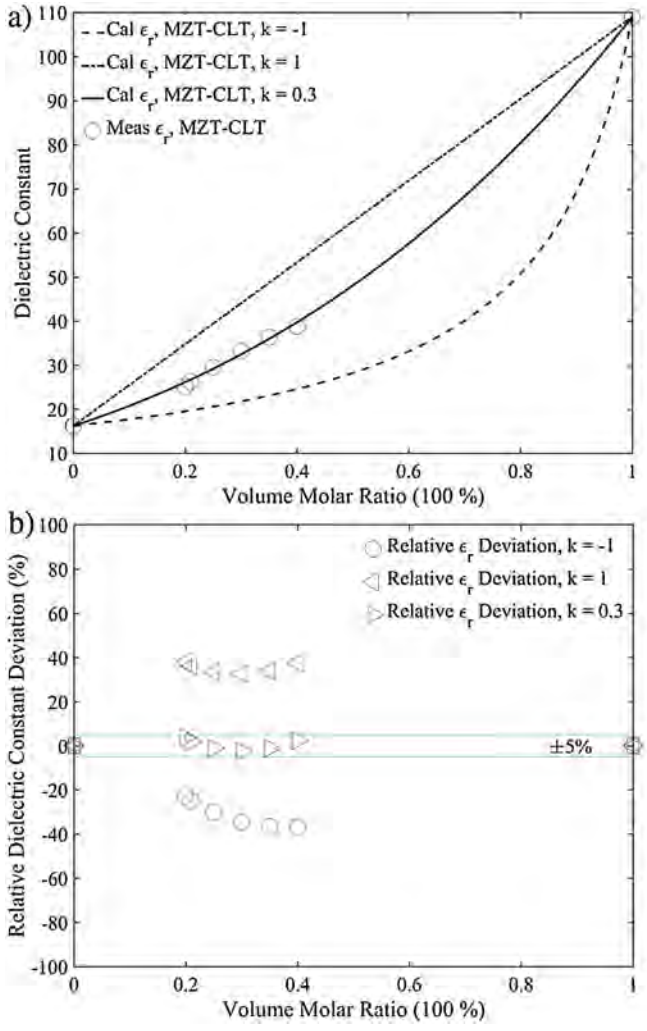

Fig. 2. (a) The example of k value determination in (1-V)$Mg_{0.95}Zn_{0.05}TiO_3$-$VCa_{0.6}La_{0.8/3}TiO_3$ (MZT-CLT): $k=-1$; $k=1$ and $k=0.3$. (b) The relative dielectric constant deviation of (1-V)$Mg_{0.95}Zn_{0.05}TiO_3$-$VCa_{0.6}La_{0.8/3}TiO_3$ (MZT-CLT) with different k values: $k=-1$; $k=1$ and $k=0.3$.

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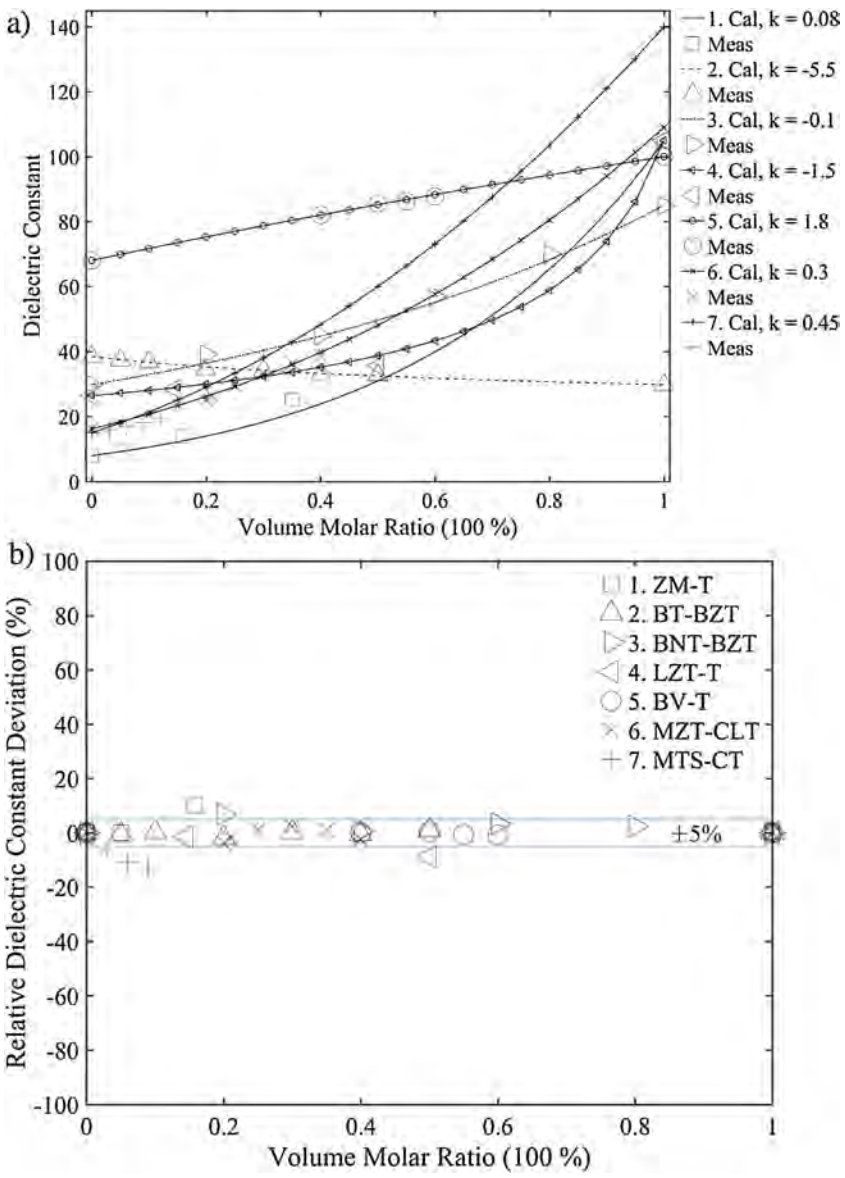

Fig. 3. (a) The calculated (Cal) and reported (Meas) dielectric constant results of: 1. (1-*V*)$ZnMoO_4$-*V*TiO_2 (ZM-T), $k = 0.08$; 2. (1-*V*)$BaTi_4O_9$-*V*$BaZn_2Ti_4O_{11}$ (BT-BZT), $k = -5.5$; 3. (1-*V*)$BaNd_2Ti_4O_{12}$-*V*$BaZn_2Ti_4O_{11}$ (BNT-BZT), $k = -0.1$; 4. (1-*V*)$Li_2ZnTi_3O_8$-*V*TiO_2 (LZT-T), $k = -1.5$; 5. (1-*V*)$BiVO_4$-*V*TiO_2 (BV-T), $k = 1.8$; 6. (1-*V*)$Mg_{0.95}Zn_{0.05}TiO_3$-*V*$Ca_{0.6}La_{0.8/3}TiO_3$ (MZT-CLT), $k = 0.3$; 7. (1-*V*)$Mg_2Ti_{0.95}Sn_{0.05}O_4$-*V*$CaTiO_3$ (MTS-CT), $k = 0.45$ versus the molar volume ratio. (b) The relative dielectric constant deviation between the reported dielectric constant data and calculated data from Eq. (6).

Therefore, we randomly set $k = -1$ and 1 to show the impact of k's sign and set $k = 1$ and 4 for example, to show the effect of k's value on Q. The quality factor ratio, R_{Q12}, and dielectric constant ratio, $R_{\varepsilon_r 21}$, between the two starting materials are randomly set as 5, 1, 1/5 and 3, 1, 1/3 respectively to show how these parameters influence the Q, in Fig. 1(a)–(c).

3. Results and discussion

Fig. 1(a) shows relative quality factor R_Q versus quality factor ratio R_{Q12} and dielectric constant ratio $R_{\varepsilon_r 21}$, versus the volume molar ratio V, for $k = -1$. When R_{Q12} is higher than 1, R_Q will increase as the volume molar ratio increases. If $R_{\varepsilon_r 21}$ is also higher than 1, R_Q shows a concave increase, meanwhile, it firstly shows a slow increase and then rapidly increases to 5, versus V. As $R_{\varepsilon_r 21}$ decreases, the concaveness of R_Q becomes more inconspicuous to linear. Until $R_{\varepsilon_r 21} \ll 1$, R_Q will show a convex increase versus V. If $R_{Q21} = 1$, the relative dielectric loss R_Q will be unity, no matter what value $R_{\varepsilon_r 21}$ is (n in Fig. 1 is 1/3, 1 or 3). These two situations correspond to $R_Q \geq 1$. Otherwise, when R_{Q12} is smaller than 1, the situation essentially is the same as $R_{Q12} > 1$ by exchanging $tan\delta_1$ and $tan\delta_2$.

Fig. 1(b) shows relative dielectric loss R_Q versus dielectric loss ratio $R_{Q12}$and dielectric constant ratio $R_{\varepsilon_r 21}$, as the volume molar ratio V changes, for $k = 1$. When $R_{Q12} > 1$, R_Q will increase as the volume molar ratio increases. If $R_{\varepsilon_r 21}$ is also larger than 1, R_Q shows a convex increase versus the V; as $R_{\varepsilon_r 21}$ decreases to 1, R_Q shows linear-like increase; when $R_{\varepsilon_r 21} < 1$, R_Q will show a concave increase versus the V. If $R_{Q12} = 1$, the relative dielectric loss R_Q also equates 1, no matter what value $R_{\varepsilon_r 21}$ is. These two situations are corresponding to $R_Q \geq 1$. For the $R_Q < 1$ part, R_{Q12} is smaller than 1 and the situation essentially is the same as $R_{Q12} > 1$ by exchanging $tan\delta_1$ and $tan\delta_2$.

Fig. 1(c) shows relative dielectric loss R_Q versus dielectric loss ratio R_{Q12} and dielectric constant ratio $R_{\varepsilon_r 21}$, as the volume molar ratio V changes, for $k = 4$. All curves show similar trend as $k = 1$ while

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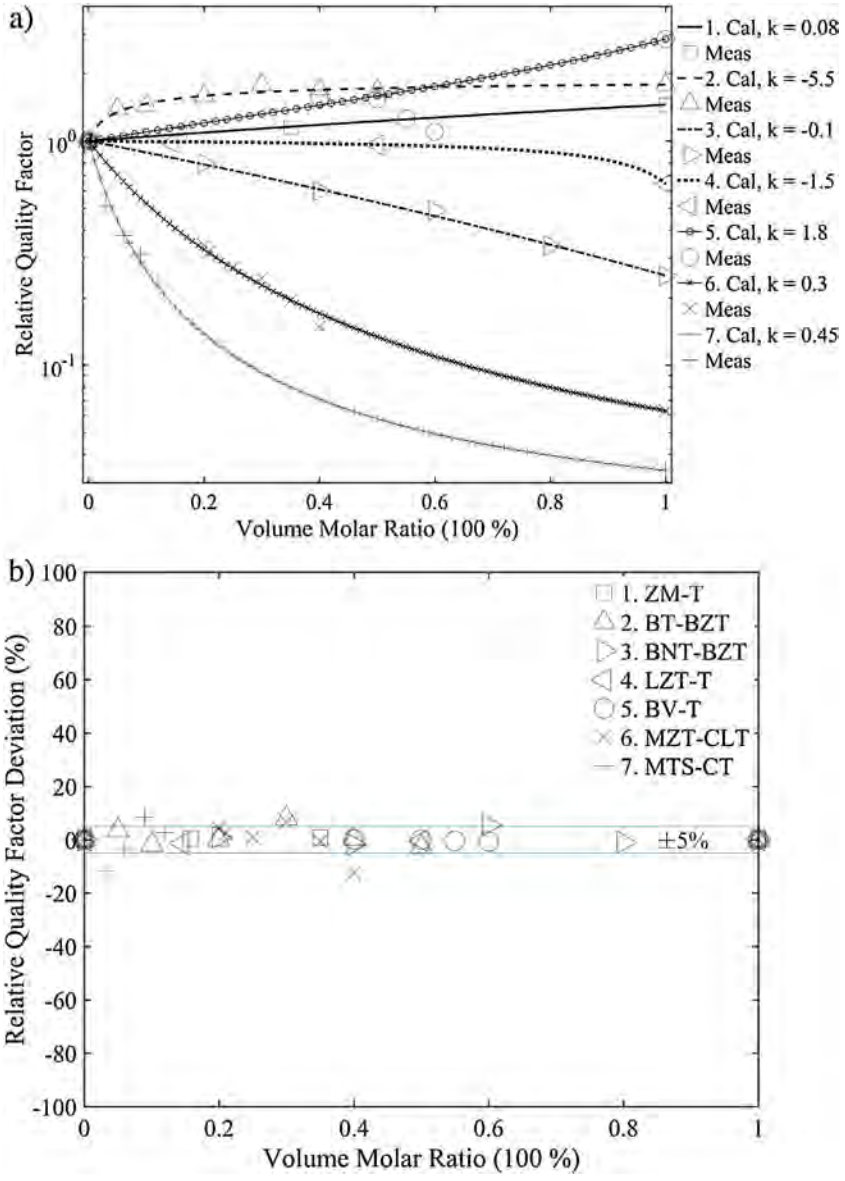

Fig. 4. (a) The calculated (Cal) and reported (Meas) relative quality factor results of: 1. (1-*V*)ZnMoO$_4$-*V*TiO$_2$ (ZM-T), $k = 0.08$; 2. (1-*V*)BaTi$_4$O$_9$-*V*BaZn$_2$Ti$_4$O$_{11}$ (BT-BZT), $k = -5.5$; 3. (1-*V*) BaNd$_2$Ti$_4$O$_{12}$-*V*BaZn$_2$Ti$_4$O$_{11}$ (BNT-BZT), $k = -0.1$; 4. (1-*V*)Li$_2$ZnTi$_3$O$_8$-*V*TiO$_2$ (LZT-T), $k = -1.5$; 5. (1-*V*)BiVO$_4$-*V*TiO$_2$ (BV-T), $k = 1.8$; 6. (1-*V*)Mg$_{0.95}$Zn$_{0.05}$TiO$_3$-*V*Ca$_{0.6}$La$_{0.8/3}$TiO$_3$ (MZT-CLT), $k = 0.3$; 7. (1-*V*)Mg$_2$Ti$_{0.95}$Sn$_{0.05}$O$_4$-*V*CaTiO$_3$ (MTS-CT), $k = 0.45$ versus the molar volume ratio. (b) The relative quality factor deviation between the reported quality factor data and calculated data from Eq. (15).

it exits some differences. When $R_{Q12} > 1$, R_Q will increase as the volume molar ratio increases. If $R_{\varepsilon_r 21}$ is also larger than 1, R_Q firstly shows a rapid increase and then smoothly increase to 5, versus *V*; as $R_{\varepsilon_r 21}$ decreases to 1, R_Q shows convex increase; when $R_{\varepsilon_r 21} << 1$,, e.g. 1/3, R_Q will show a concave increase versus *V*. If $R_{Q12} = 1$, the relative dielectric loss R_Q equates 1, no matter what value $R_{\varepsilon_r 21}$ is. For $R_Q < 1$, in other words, $R_{Q12} < 1$, the situation essentially is the same as $R_{Q21} > 1$ by exchanging $tan\delta_1$ and $tan\delta_2$.

Though some differences between Fig. 1(b) and (c) exist, their varying trends are actually similar, while for Fig. 1(a) which possesses a negative *k* value, it illustrates totally different variation curve. For different sign of *k*, −1 and 1, when $R_{\varepsilon_r 21}$ and R_{Q12} are the same, 3 and 5, if *k* is negative, the quality factor shows a concave increase curve and if *k* is positive, it shows a convex increase trend. For different value of *k*, 1 and 4, when $R_{\varepsilon_r 21}$ and R_{Q12} are the same, 3 and 5, if *k* is small, the quality factor shows a relative smooth increase curve while if *k* is large, it firstly shows a rapid increase and then keeps nearly at a fixed value. Therefore, both the sign and absolute value of *k* impacts the way of how quality factor varies and for a fixed *k*, the quality factor will be determined by the dielectric constant and quality factor of the starting materials.

In the precedent discussion, the value of *k* is directly given, so in the following the determination of *k* value of (1-*V*) $Mg_{0.95}Zn_{0.05}TiO_3$ – *V* $Ca_{0.6}La_{0.8/3}TiO_3$ will be shown as an example [12]. The relative dielectric constant deviation, typically less than 10%, will be given to confine the *k* value of a system:

$$R_{\varepsilon_r - deviation} = \frac{R_{\varepsilon_r - calculated} - R_{\varepsilon_r - reported}}{R_{\varepsilon_r - calculated}} \times 100\%. \quad (16)$$

As shown in Fig. 2(a), putting dielectric constant of two starting ceramics and random *k* values of −1 and 1 into Eq. (6), the deviation is large in Fig. 2(b). Continuously adjusting *k* value to 0.3, the $R_{\varepsilon_r - deviation}$ of most data approaches near 0%. Then this *k* of 0.3 could be applied to Eq. (15) to calculate the quality factor of the two-phase system. By the same way, *k* values of different groups can be determined.

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In the following, more examples will be given to show the effectiveness of Eq. (15) for the quality factor calculation. There are so many reports on multiphase quality factor calculation and we cannot figure them out one by one. The dielectric constant in the range of 10–140 of 7 typical groups are shown as examples. These typical groups are: $MgTiO_3$, $BaZn_2Ti_4O_{11}$, $BaTi_4O_9$, $Ba_{6-3x}Ln_{8+2x}Ti_{18}O_{54}$, TiO_2, and $CaTiO_3$ (Ln represents rare earth elements) et al. based ceramics [4–6,8,9,11–13].

In most reports, only data of *Qf* values are given. We assume that the samples' dimension is stable in each report. From Ref. [17], the resonant frequency is reversely related to the size of the cylinders and dielectric constant. In order to precisely extract the *Q* from these data, we will take the dielectric constant into consideration and assume a constant size of their samples, to calculate the resonant frequency (*f*):

$$f \propto \frac{1}{\sqrt{\varepsilon_r}} \tag{17}$$

Eq. (17) actually treats other parameters as a constant for each group of material.

We will firstly get the *k* values from the reported dielectric constant data according to Eq. (6). In Fig. 3(a), the results of calculated and reported dielectric constant data of 7 different groups are shown. Most calculated data fit well to the reported data, with typical relative dielectric constant deviation around or less than ±5% in Fig. 3(b). In Fig. 3(a), "Cal" means calculated data and "Meas" equates the measured data in literatures [7–13].

Then applying these *k* values to Eq. (15), quality factor results of 7 typical two-ceramic-mixtures will be depicted: 1. (1-*V*)$ZnMoO_4$-*V*TiO_2, $k = 0.08$; 2. (1-*V*)$BaTi_4O_9$-*V*$BaZn_2Ti_4O_{11}$, $k = -5.5$; 3. (1-*V*)$BaNd_2Ti_4O_{12}$-*V*$BaZn_2Ti_4O_{11}$, $k = -0.1$; 4. (1-*V*)$Li_2ZnTi_3O_8$-*V*TiO_2, $k = -1.5$; 5. (1-*V*)$BiVO_4$-*V*TiO_2, $k = 1.8$; 6. (1-*V*)$Mg_{0.95}Zn_{0.05}TiO_3$-*V*$Ca_{0.6}La_{0.8/3}TiO_3$, $k = 0.3$; 7. (1-*V*)$Mg_2Ti_{0.95}Sn_{0.05}O_4$-*V*$CaTiO_3$, $k = 0.45$ versus *V* [7–13]. In Fig. 4(a), "Cal" means calculated data and "Meas" equates the measured data in literatures. The relative quality factor deviation, typically less than ±10%, will be given to check the *k* value of a system:

$$R_{Q-deviation} = \frac{R_{Q-calculated} - R_{Q-reported}}{R_{Q-calculated}} \times 100\%. \tag{18}$$

The relative quality factor deviation data are shown in Fig. 4(b) to confirm the effectiveness of Eq. (15).

In Fig. 4(a), the reported quality factor fits well with the calculation and in Fig. 4(b), the relative quality factor deviation is around ±5%. In practice, once the relative quality factor of the multiphase is determined, the quality factor could be obtained by Eq. (11). As a result, with the properties of the two starting materials, we can precisely predict the quality factor of the multiphase mixtures, without considering the microstructures. In other words, from Eq. (15), if the ceramic mixtures are well sintered, what the change of the microstructure actually influencing is the dielectric constant [7–13].

4. Conclusions

For the first time, in this paper, we derived a precise *Q* calculation formula for multiphase ceramic mixtures and the effectiveness the formula in the two-phase-ceramic mixtures has been confirmed. It is found that the quality factor of mixtures is not only determined by each component's quality factor, but also related to the dielectric constant and the *k* value.

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