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Reply to Comment on "Chemical-Composition-Dependent Metastability of Tetragonal ZrO_2 in Sol–Gel-Derived Films under Different Calcination Conditions"

The comment given by Khajavi and Baboluo[1] raises the concern about the calculation procedure published in our paper for estimating phase compositions of zirconia films.[2] In the comment, they indicate that our paper uses an inappropriate procedure to calculate the volume fractions of tetragonal and monoclinic phases. In addition, Khajavi and Baboluo suggest that the method proposed by Toraya et al.[3] is the way that is more capable of achieving true results.

We thank the authors for commenting on XRD analysis of ZrO_2 phases. Moreover, the detailed review on calculating models provided by the authors is highly appreciated. In our published paper,[2] we calculated the volume fraction of tetragonal and monoclinic phases based on the empirical equations[4]

$$X_t = \frac{I_t(101)}{I_t(101) + I_m(111) + I_m(\bar{1}11)} \quad (1)$$

$$X_m = 1 - X_t \quad (2)$$

where the $I_t(101)$, $I_m(111)$, and $I_m(\bar{1}11)$ represent the intensities of the diffraction peaks along the (101) plane of the tetragonal phase and the (111) and the $(\bar{1}11)$ planes of the monoclinic phase, respectively. Because of not considering structure factors, the values calculated based on the empirical equation have as much as 20% deviation from actual ratios. Many literatures have referred this equation to estimate the volume fraction for these two phases.[5] Although the calculation from empirical equation only gives approximate results, it is not a wrong procedure as mentioned by Khajavi and Baboluo in their comment.

We agree with that the more accurate ratios of tetragonal and monoclinic phases can be obtained from the modified equation[3]

$$v_m = \frac{1.311X_m}{1 + 0.311X_m} \quad (3)$$

$$v_t = 1 - v_m \quad (4)$$

where v_m and v_t are the volume fraction of a monoclinic and a tetragonal phase, respectively. Based on the modified equation, we recalculate the volume fractions of the tetragonal and monoclinic phases, and the results together with our published data are listed in Table 1. The volume fractions of the monoclinic phase published in our paper are in the range of 0.65–0.96. These values are only 1.0–8.0% lower than those (0.71–0.97) calculated using the modified equation, which clearly indicate the satisfactory results obtained from the empirical equation. In our published paper, we mainly investigated the meta-stability of a tetragonal ZrO_2 and the mechanism of tetragonal-to-monoclinic phase transformation under different atmospheres based on the correlation between the phase composition and the O/Zr ratios of ZrO_2 films. The deviations of the empirical data from the modified results do not influence the conclusion in our published paper.

Table 1. Volume Fraction of Tetragonal and Monoclinic Phases Calculated Using Modified and Empirical Equations

samples	modified equation v_t	modified equation v_m	empirical equation X_t	empirical equation X_m
ZrO_2-550-air[a]	0.29	0.71	0.35	0.65
ZrO_2-700-N_2[b]	0.03	0.97	0.04	0.96
ZrO_2-950-N_2[b]	0.12	0.88	0.15	0.85

[a]The ZrO_2 film calcined at 550 °C in air, [b]means the ZrO_2 film calcined at 700 °C (or 950 °C) in N_2.

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Notes

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