Supplementary material (ESI) for Journal of Materials Chemistry

Supporting information for:

Zero thermal expansion in the (1-*x*)$PbTiO_3$-*x*$Bi(Mg,Ti)_{1/2}O_3$ piezoceramics

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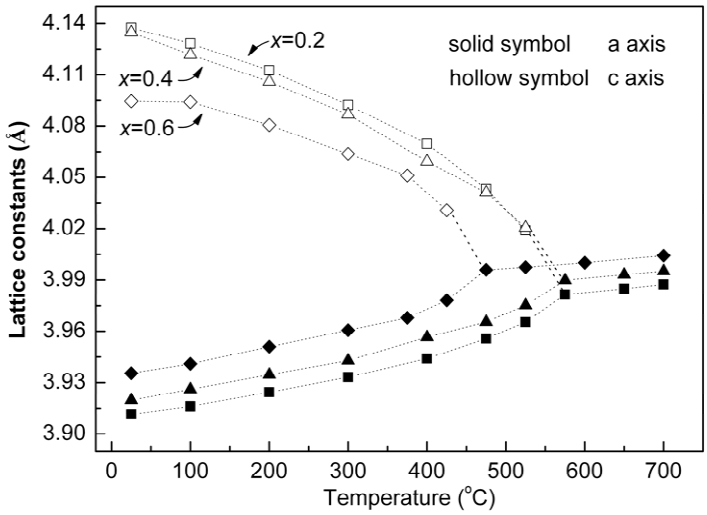

Figure S1. Unit cell volumes of (1-*x*)$PbTiO_3$-*x*$Bi(Mg,Ti)_{1/2}O_3$ (*x*=0.2、0.4、0.6) as function of temperature in the range of 25-700°C.

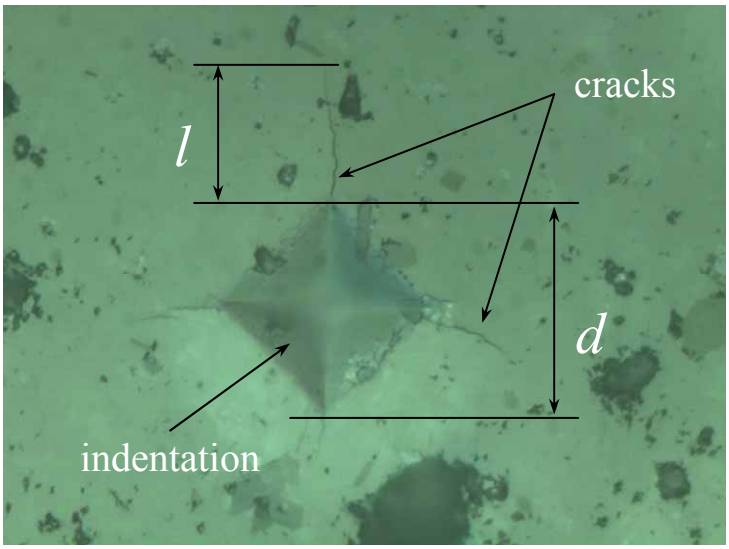

Figure S2. A typical photo taken by microscope camera in the Vickers indentation hardness measurement. The fracture toughness (K_{IC}) of the ceramics were characterized by indentation method carried on the Digital Microhardness tester (HVS-1000) with different loads and 20 s of dwell time. After loading, there would be indentation on the surface of the ceramics, and there were cracks extended from the indentation's tips.The hardness could be directly numerated from the instrument and the K_{IC} were calculated by following equation

$$K_{IC} = \frac{0.0624P}{dl^{1/2}}$$

where *d* is diagonal length of the indentation, *l* is the crack's vertical length measured from the tip of indentation. The *d* and *l* were measured directly from the photos taken by microscope camera. Generally, the longest crack was measured for the *l* magnitude. The K_{IC} obtained under different loads were counted for the average and exhibited in figure 5b, the error limits showed the results'

distribution.

Generally, the intrinsic thermal expansion α_V and the apparent thermal expansion α_l meet the relationship: $\alpha_V \approx 3\alpha_l$ which derived from the following computations:

For $\alpha_V = \frac{1}{V_0}\frac{dV}{dT}$, $\alpha_l = \frac{1}{l_0}\frac{dl}{dT}$ where V is the unit cell volume, l is the one-dimensional length of the ceramic sample, T is the temperature. Actually, the samples measured in the dilatometer were club-shaped ceramics, which were pressed and sintered from the finished powder. Because there were unit cells in any orientation, the ceramic samples could be considered as isotropic; consequently, the thermal expansion would be isotropic as well. Thus, the apparent thermal expansion was independent of the shape of the samples. The volumetric thermal expansion is certainly proportional to the one-dimensional thermal expansion.

Define $V_1=l^3$, ignoring the sintered defects in the ceramics, $V_1=k\cdot V$ (k is a coefficient which can be interpreted as the quantity of the unit cells a sample which volume is V_1 contains). In the actual samples, considering the pore, the k will be a little bigger.

$$\alpha_V = \frac{1}{V_0}\frac{d(V)}{dT} = \frac{k}{V_{1_0}}\frac{d(\frac{V_1}{k})}{dT} = \frac{1}{V_{1_0}}\frac{d(V_1)}{dT} = \frac{1}{l_0^3}\frac{d(l^3)}{dT} = \frac{1}{l_0^3}\frac{3l^2dl}{dT} \approx \frac{3}{l_0}\frac{dl}{dT} = 3\alpha_l \quad (l_0 \approx l)$$