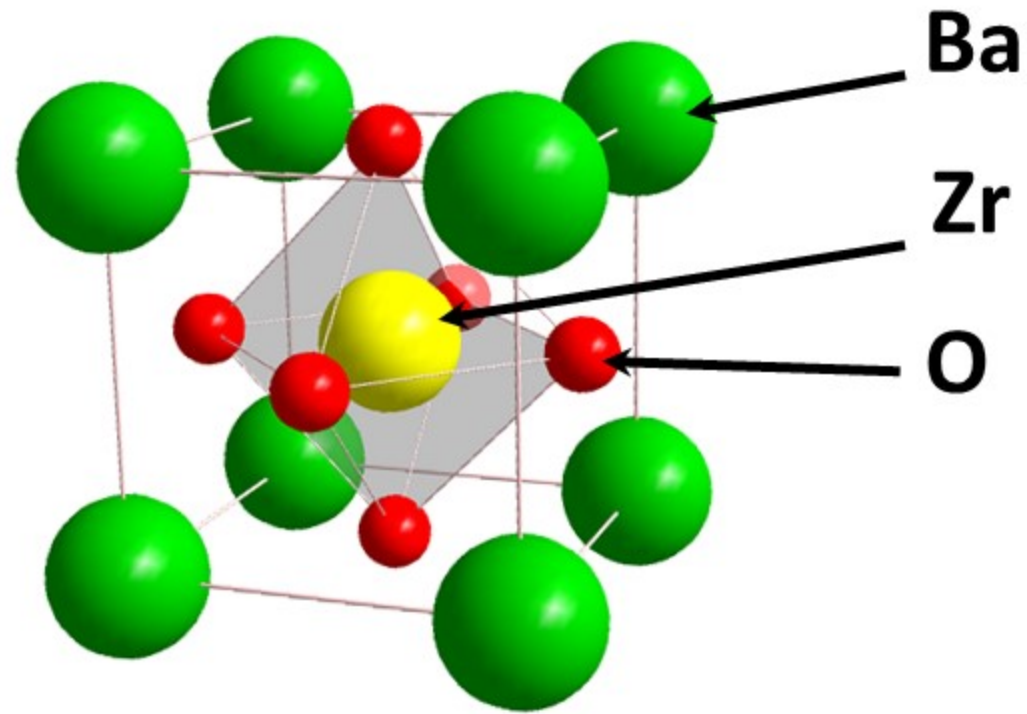


# Large Lattice Constant and Large Band Gap Cubic Perovskite: BaZrO<sub>3</sub> Single Crystal

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# Cubic Perovskite BaZrO<sub>3</sub>

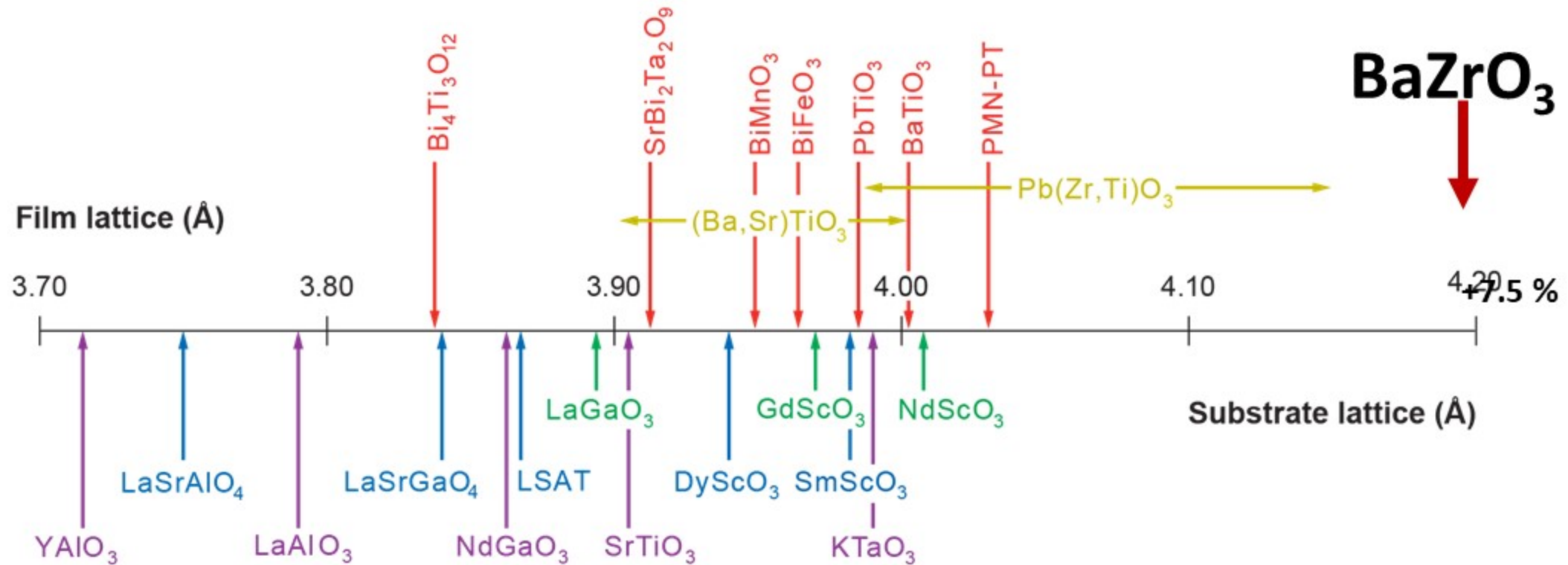


**Structure : Cubic (P m -3 m)**

**Lattice Constant : 4.2039 Å**

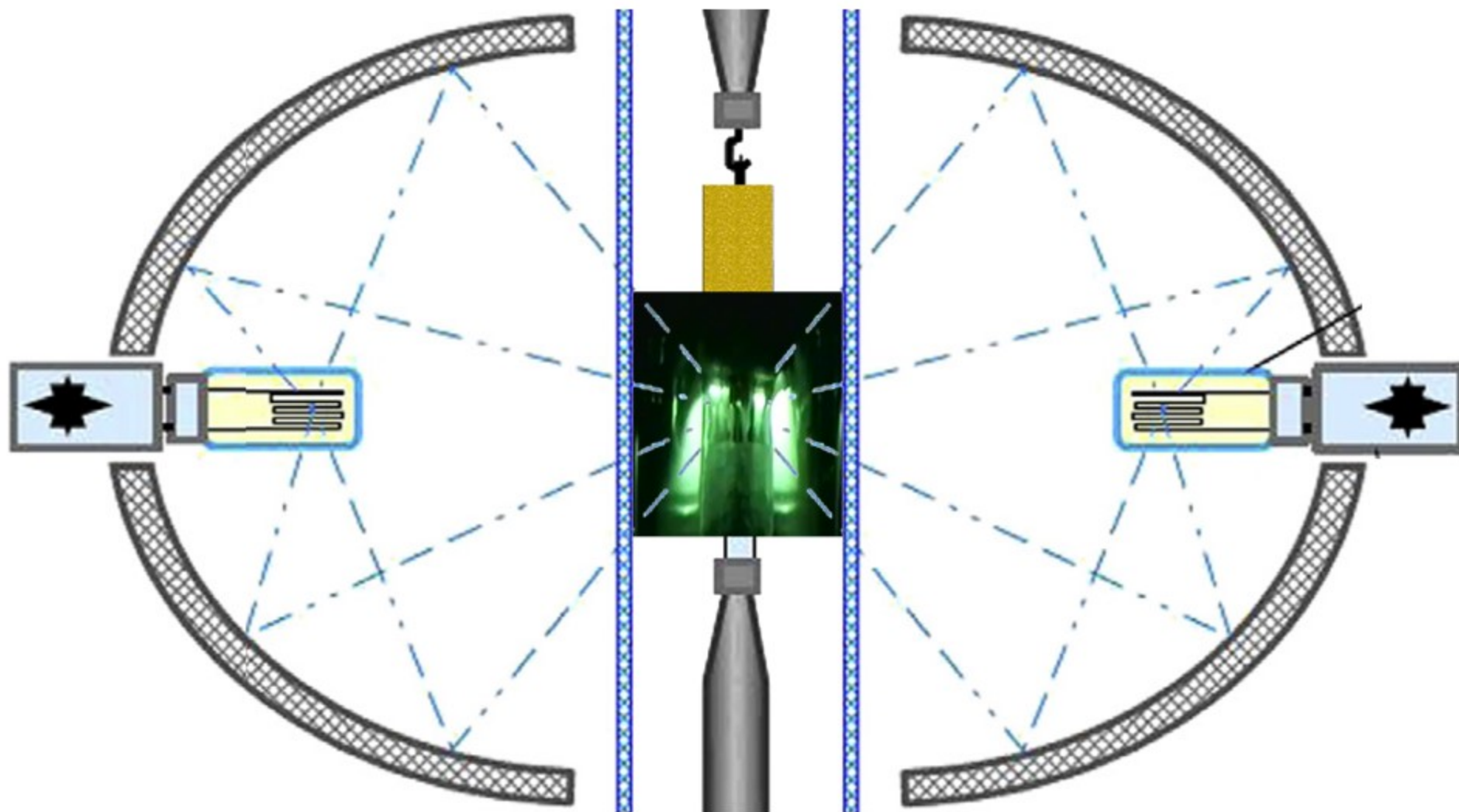
**Melting Temperature : 2500-2700 °C**

# Pseudocubic Lattice Constants of Perovskites

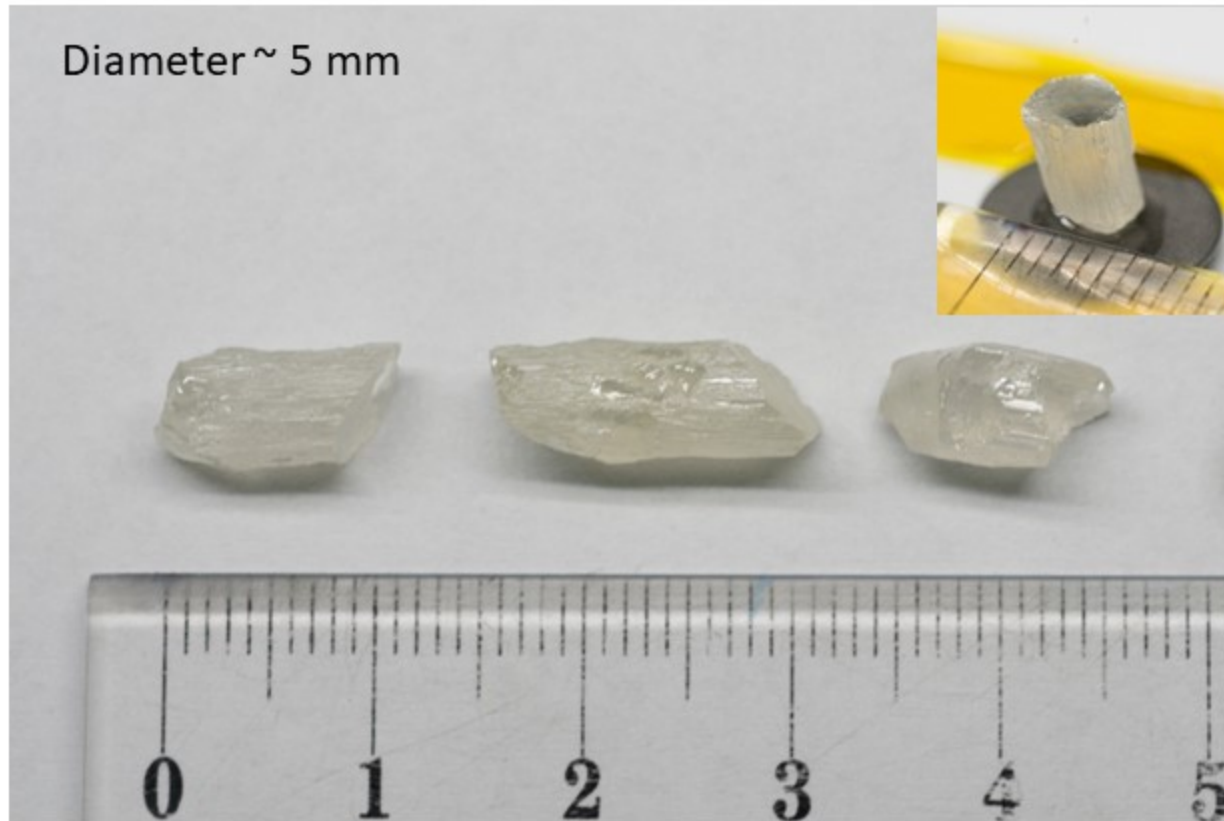




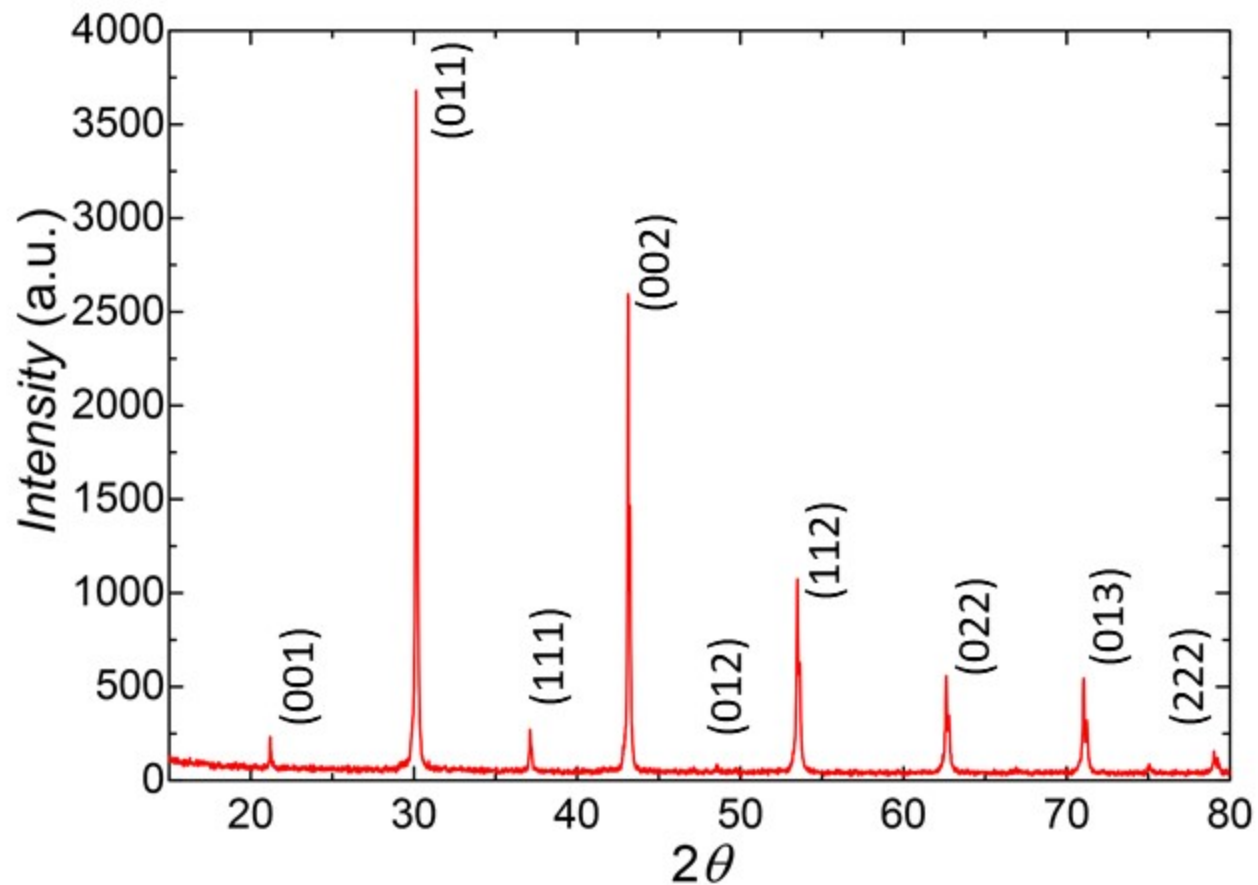
## Optical Floating Zone Method



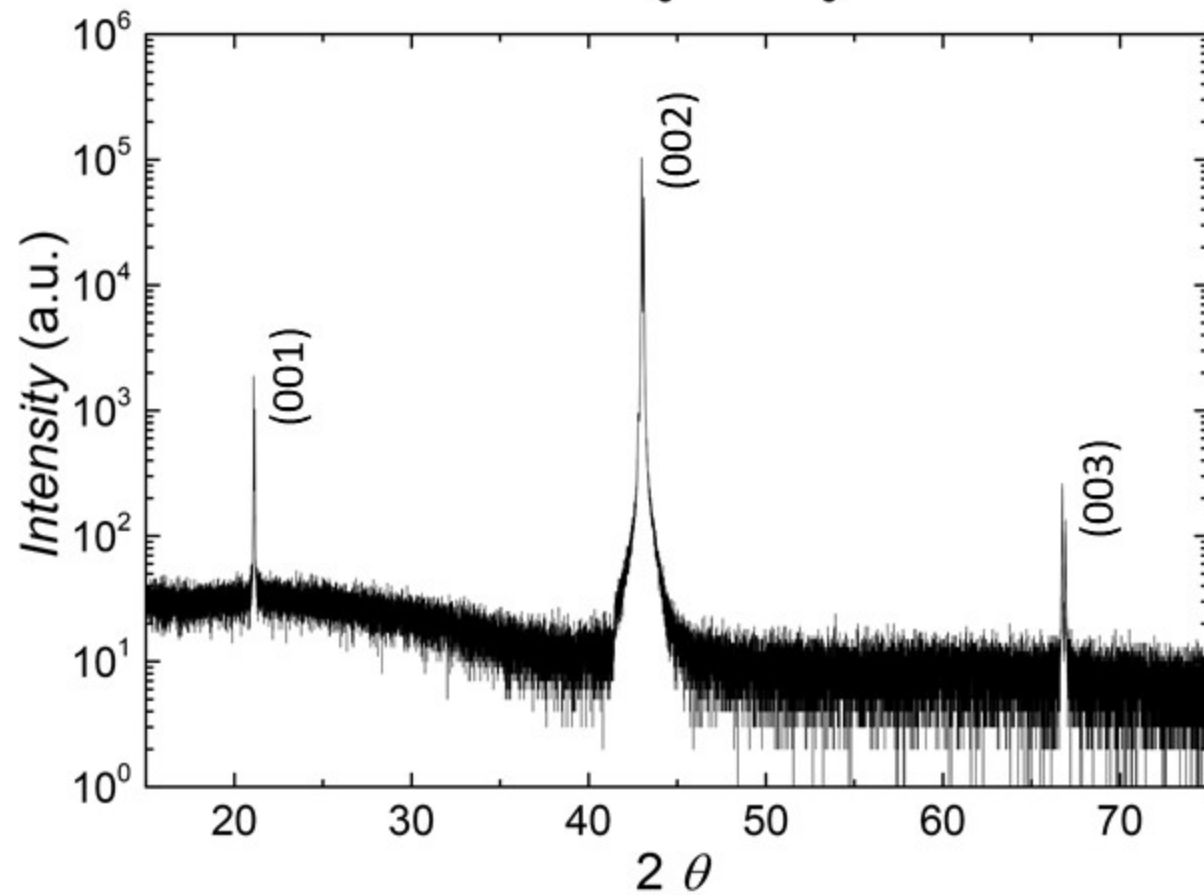
# BaZrO<sub>3</sub> Single Crystal



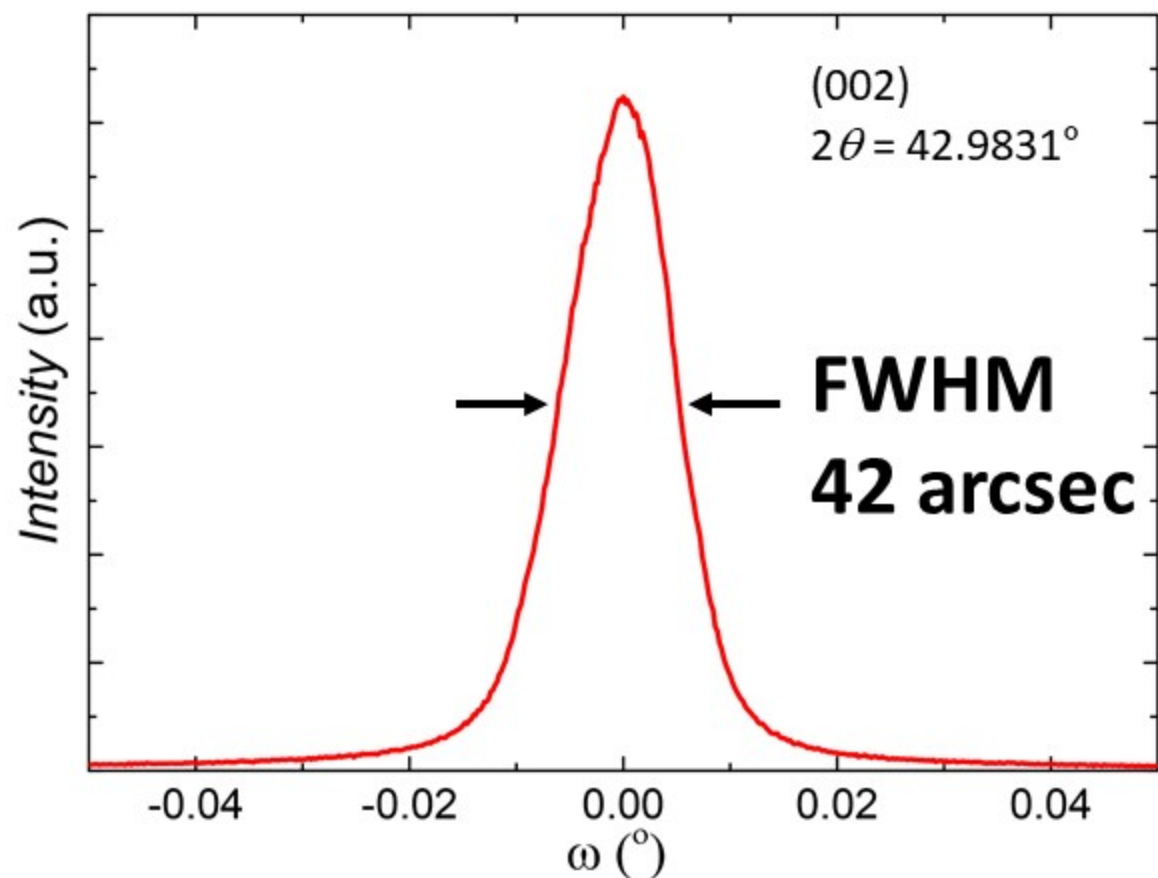
## Powder XRD



## HR-XRD on (001) surface



## Rocking Curve

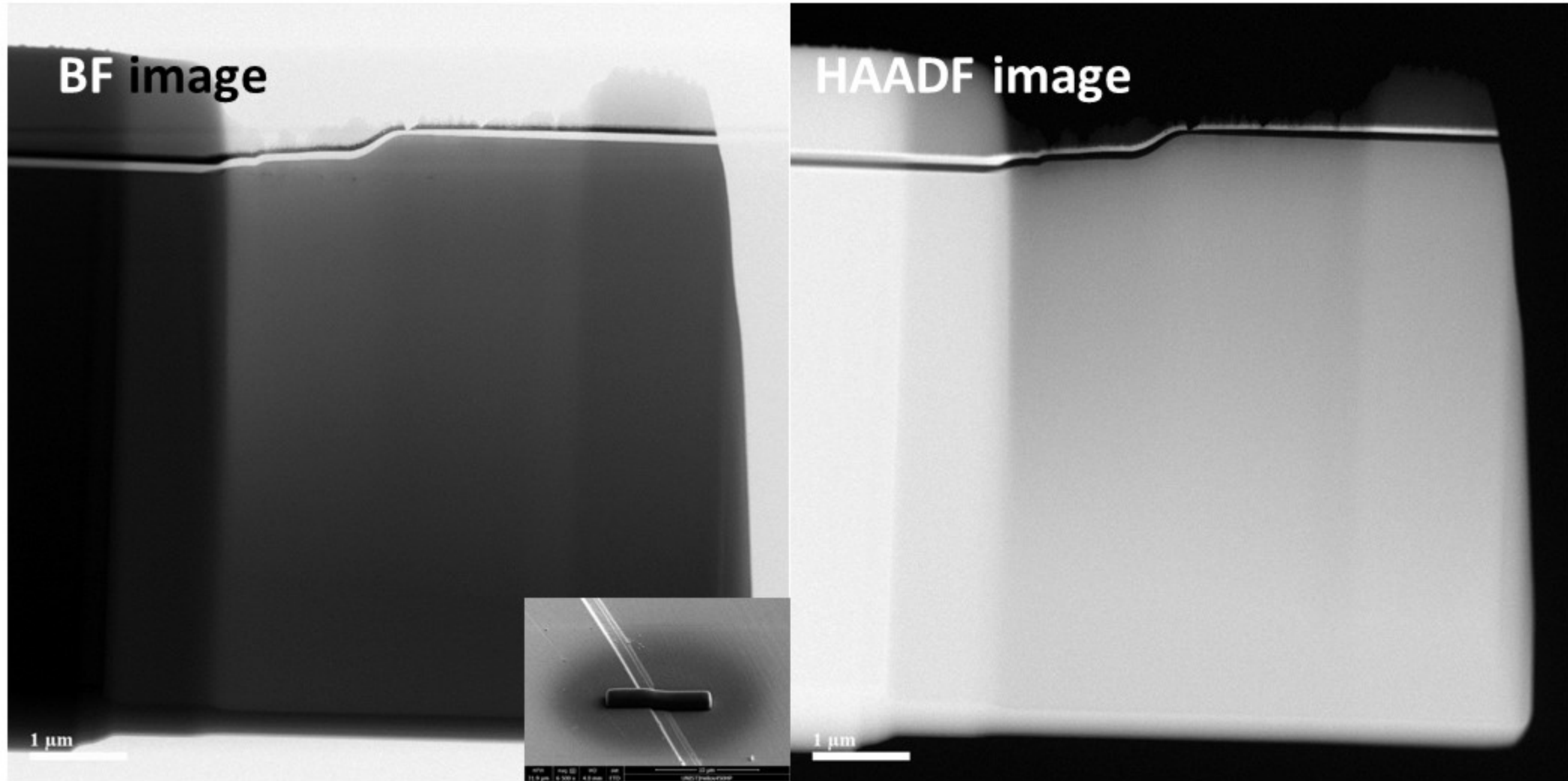


Crystal	FWHM (arcsec)	Thin film	FWHM (arcsec)
$\text{SrTiO}_3^{1)}$	126	$\text{SrTiO}_3^{6)}$	15
$\text{BaTiO}_3^{2)}$	319	$\text{Fe}_2\text{O}_3^{7)}$	432
$\text{ZnO}^{3)}$	12	$\text{ZnO}^{8)}$	28
$\text{LiTaO}_3^{4)}$	1440	$\text{NiO}^{9)}$	72
$\text{Al}_2\text{O}_3^{5)}$	720	$\text{SiO}_2^{10)}$	15

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- 8) Q.-X. Yu, et al., Chin. Phys. Lett. 20, 12 (2003)
- 9) E. Lindahl, Digital Comprehensive Summaries of Uppsala Dissertations from the Faculty of Science & Technology 701, (2009)
- 10) S.-Y. Matsuno, et al., Analytical and Computational Science Laboratories, Asahi Chemical Industry Co, Advances in X-ray Analysis, Vol.43

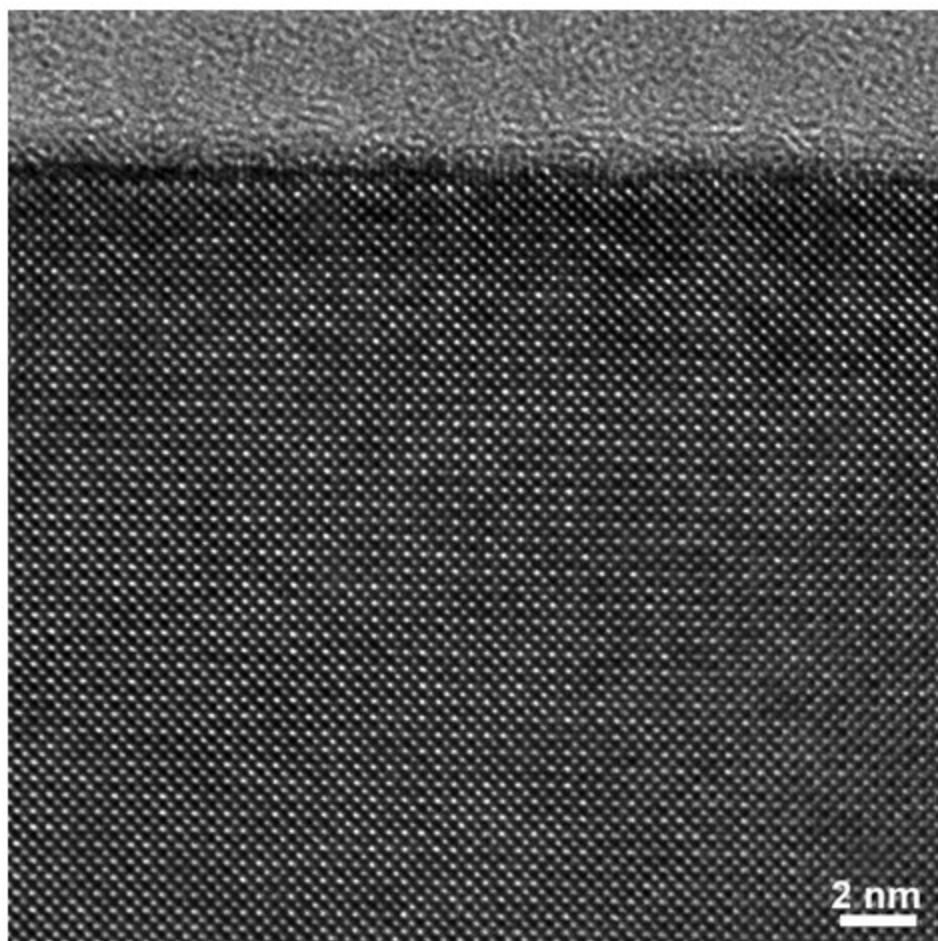


## Scanning Transmission Electron Microscopy

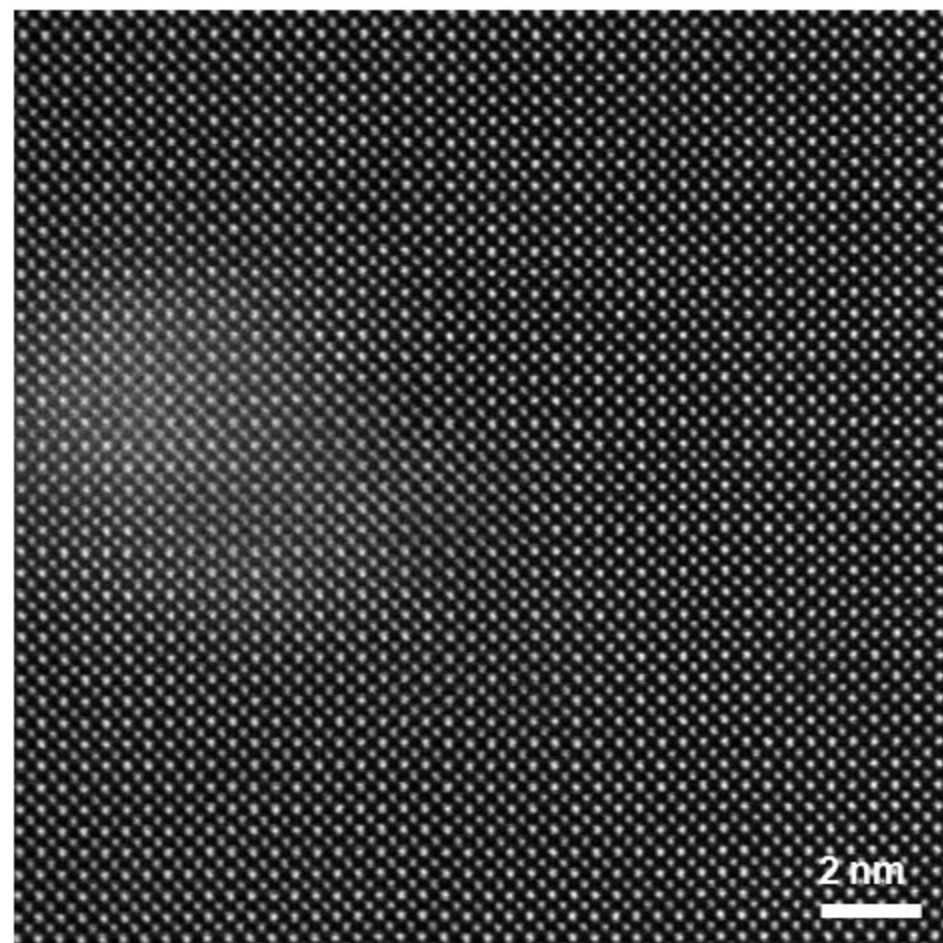




## HRTEM



## HAADF-STEM



1. Using the optical floating zone method,  $\text{BaZrO}_3$  single crystal is successfully grown.
2. The grown single crystal has cylindrical shape with diameter of 5 mm and length of  $\sim 1$  cm.
3. Lattice constant of our  $\text{BaZrO}_3$  single crystal is 7.5 % larger than that of  $\text{SrTiO}_3$ .
4. In study of the rocking curve, the Full Width at Half Maximum (FWHM) of the (002) peak is 42 arcsec.  
It indicates that our  $\text{BaZrO}_3$  single crystal has high quality in terms of crystallinity.
5. Cleaved (001) surface has atomically flat surface and shows clear step terraces with width of 5  $\mu\text{m}$ .
6. Our TEM studies represents that our  $\text{BaZrO}_3$  single crystal has no structural defect. Ba and Zr atoms are well ordered.
7. In ultraviolet-visible-near-infrared transmission spectra, it's found energy band gap of  $\text{BaZrO}_3$  is 5.0 eV.