

Atomic structures for ABO₃ perovskite

Zhadyra Zakiyeva¹, Aisulu Abuova² Diana Nygmetzhanova³

¹ L.N. Gumilyov Eurasian National University, Astana, Kazakhstan

² L.N. Gumilyov Eurasian National University, Astana, Kazakhstan

³ L.N. Gumilyov Eurasian National University, Astana, Kazakhstan

Barium titanate - perovskite was discovered half a century ago, but due to its unique crystal structures, physical and chemical properties, the material still attracts a lot of attention of researchers. In addition, barium titanate has a high dielectric constant, and their excellent piezoelectric and ferroelectric properties are also known. Over the past decade, it has become one of the important materials with excellent dielectric, ferroelectric and piezoelectric properties, due to which this type of material has great capabilities, which allows them to be used in the production of electronic devices. It is one of the most thoroughly studied cubic perovskites, and has paraelectric properties at high temperatures and has a simple cubic perovskite structure. Most of the ABO₃ type perovskites have the same stable phases at different temperatures.

Perovskites can exist in various phase modifications, which generally exhibit different properties. The number of phase modifications depends on the specific combination of A and B cations [1, 2]. Many perovskites, specifically, demonstrate the presence of other phases. The highly symmetrical cubic phase of the *Pm-3m* crystal is also stable at high temperatures and demonstrates a series of three phase transitions with decreasing temperature: tetragonal *I4/mcm* at 393 K, orthorhombic *Amm2* at 278 K and rhombohedral *R3m* at 183 K, as shown in Figure 1.

Over the past 20 years, several first principles calculations have been carried out, in which more attention was paid to the structural and electronic properties of the four phases [3]. Perovskites are complex oxides, mainly of the composition ABO₃, where A is a divalent metal, and B is a tetravalent (transition) metal. DFT calculations are carried out with high accuracy to precisely obtain ferroelectric phases. Minimization is not required for a cubic structure. The tetragonal structure was optimized by changing the coordinates of the ions, since the symmetry (distortion in the z direction) allows optimization in a fixed *c/a* ratio, while maintaining a fixed volume. The theoretical study of this perovskite still requires detailed analysis, since it does not show the same result compared to experimental data and still remains an object research. Experimental data showed band gap widths of about 3.7 eV for the cubic phase and 3.9 eV for the tetragonal phase. In general, density functional theory (DFT) will be applied with a combination of different approximations to describe the structure of the perovskite band gap.

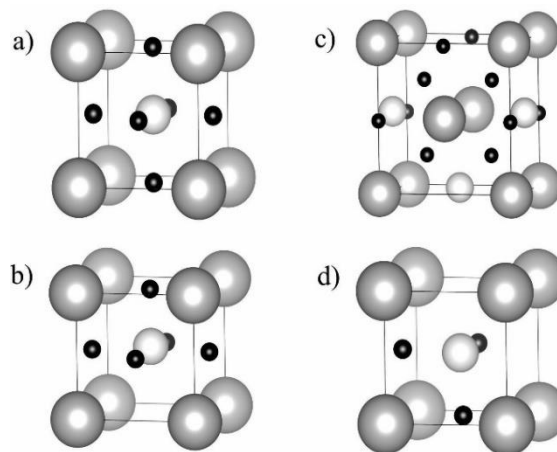


Figure 1. Unit cells *BaTiO₃* in cubic, tetragonal, orthorhombic and rhombohedral phases.

Then, using the optimized coordinates of the ion particles, the relation (maybe the ratio) c/a was optimized at a constant volume. Thus, the relation $Ti(1/2, 1/2, 1/2 + \Delta z_{Ti})$, $O_1(1/2, 1/2, \Delta z_{O_1})$, $O_2(1/2, 0, 1/2 + \Delta z_{O_2})$ it has been optimized while minimizing. The lattice parameters were also optimized in the orthorhombic phase: a, b, c and $Ti(1/2, 0, 1/2 + \Delta z_{Ti})$ $O1(0, 0, 1/2 + \Delta z_{O1})$, $O2(1/2, 1/4 + \Delta y_{O2}, 1/4 + \Delta z_{O2})$. Lattice parameter a ($a = b = c$), angle α ($\alpha = \beta = \gamma$) $\Delta Ti(1/2 + \Delta x, 1/2 + \Delta x_{Ti}, 1/2 + \Delta x_{Ti})$ $O(1/2 + \Delta x_O, 1/2 + \Delta x_O, 0 + \Delta z_O)$ were optimized values for the rhombohedral phase.

Acknowledgements

The work was carried out with the financial support of the Ministry of Science and Higher Education of the Republic of Kazakhstan, grant IRN AR14869492 "Development of nanocrystalline metal oxide catalysts for hydrogen production".

References

- [1] Steele, C.H., & Heinzel, A. Materials for fuel-cell technologies, *Nature*, 414, 345-352 (2001)
- [2] Woodward, P.M. Octahedral tilting in perovskites. II Structure stabilizing forces. *Acta crystallographica*, 53, 44 (1997)
- [3] Holm, B., Ahuja, R., Yourdshabyan, Y., Johanson, B., & Lundqvist, B.I. *Phys. Rev.*, 59, 12777 (1999)



Zhadyra Zakiyeva 3 rd year doctoral student «Technical Physics», L.N. Gumilyov Eurasian National University, K. Munaitpasov St. 13, Astana, Kazakhstan.

Zhadyra Zakiyeva, e-mail: zhadyrazakiyeva@gmail.com tel: +7 777 309 01 20