

STUDY OF TITANIUM AND OXYGEN IONS CHARGE IN SOME FERROELEKTRICS AND SIMILAR TO THEM OBJECTS

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The objects of study were isostructural substances $ATiO_3$ ($A = Ca, Sr, Ba, Cd, Pb$) and oxide TiO_2 , used in their synthesis. $BaTiO_3$ and $PbTiO_3$ are the ferroelectrics. $SrTiO_3$ is virtual ferroelectric. Ferroelectrics are widely used in different regions of electro- and radiotechniques. Therefore, the study of electronic structure and chemical bond features in these substances is important.

In this work by X-ray photoelectron spectroscopy were received data on the binding energy of the core levels of titanium and oxygen $ATiO_3$ and TiO_2 . The spectra were obtained by HP5950 spectrometer.

Measurements show that the increase in the atomic number of the first component in $ATiO_3$ rather weakly affects the position of titanium and oxygen levels in these substances. At the same time the positions of these levels in the oxide TiO_2 differs from that of $ATiO_3$. The direction of chemical shift of these levels indicates that the Ti-O bond in $ATiO_3$ has more covalent character than in TiO_2 .

The $TiL\alpha$ - and $OK\alpha$ -X-ray were also obtained for all studied substances. $TiL\alpha$ - spectra characterized the Ti 2p- electrons distribution in a valence band. $OK\alpha$ -spectra characterized, respectively, O 2p- electrons distribution. $OK\alpha$ -spectra in $ATiO_3$ substances and TiO_2 are presented at the figure.

The energy position of the $TiL\alpha$ - and $OK\alpha$ -spectra maxima slightly varies with the atomic number of the first component in $ATiO_3$. The direction and value of these maximums shift in $ATiO_3$ relatively TiO_2 indicates some increase in the degree of covalence of Ti-O bond in $ATiO_3$.

The results are interpreted on the basis of the analysis of the crystal structure of substances.

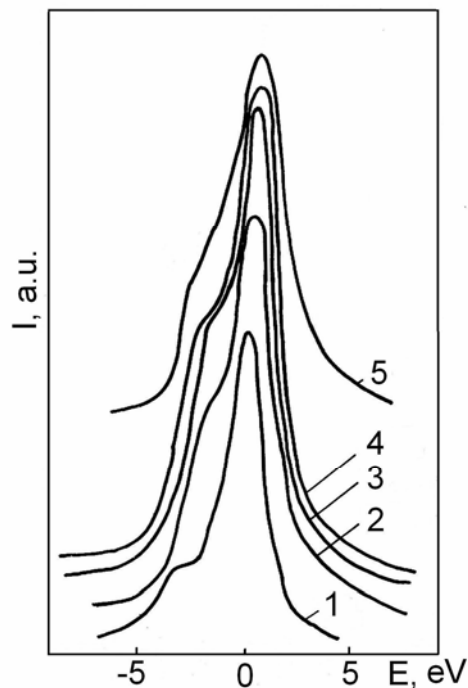


Fig. $OK\alpha$ - spectra for substances of $ATiO_3$ and TiO_2 : 1 - TiO_2 , 2 - $CaTiO_3$, 3 - $BaTiO_3$, 4 - $SrTiO_3$, 5 - $PbTiO_3$. Energy of the TiO_2 band maximum is taken as zero

Conclusions:

1. The titanium and oxygen ions charge differs slightly when A-component in $ATiO_3$ ($A = Ca, Sr, Ba, Cd, Pb$) differs.
2. Degree of covalence of the Ti-O bond in $ATiO_3$ more than in TiO_2 . These results are supported by studies of these compounds by the X-ray photoelectron spectroscopy and X-ray spectroscopy methods.