

Coordination compounds - precursors for the synthesis of barium and strontium titanates by MOCVD– technique

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The compounds for the production of BaTiO₃ and SrTiO₃ thin films were investigated by experimental and theoretical methods (the structural-thermochemical approach), the conditions of their transfer into the gas phase were determined. The thermochemistry of the vaporization of these complexes was examined.

In order to obtain barium and strontium titanates by MOCVD – technique, conformational analysis of the molecular design of strontium, barium-bearing compounds (earlier titanium [I]) potentially containing a little number of intermolecular interactions, was conducted (analysis of steric difficulties, the number and types of thermochemically significant intermolecular contacts). As titanium - containing precursors - bis[(μ-N-methyldiethoxoamine)bis(2,3-dimethyl-2,3-butanediolate)titanium](I) and bis[(μ-N-ethyldiethoxoamine)bis(3,4-diethyl-3,4-hexanediolate)titanium](II) were chosen.

Crown-β-diketonates [Sr(15C5)(C₅O₂F₆H)₂](III) and [Ba(18C6)(C₅O₂F₆H)₂](IV) (-C₅O₂F₆H – 1,1,1,5,5,5-hexafluoro-2,4-pentanedionato-group) were used as Sr and Ba - bearing precursors. Evaporation enthalpies (I – IV) were calculated by summing the contributions from the individual groups. Addition of the measured melting enthalpies gave sublimation enthalpies of I and II, agreeing closely with data determined experimentally by using high temperature mass spectrometry.

Experimental values of the evaporation enthalpies of III and IV exceed the corresponding theoretical values, obtained using the group contributions method. It is supposed, that the additional intermolecular interactions involving oxygen atoms of crown-ether groups, which are the most mobile ones.

The possibility of the synthesis of binuclear Ti - Ba (Sr) - containing volatile molecular compounds was investigated and discussed. Thin films of TiO₂, BaTiO₃, SrTiO₃ were obtained using MOCVD - technique.

References

1. D.V. Sevast'yanov, V.G. Sevast'yanov, E.P. Simonenko, T. Kemmitt, G.J. Gainsford, N.T. Kuznetsov, *Thermochimica Acta*, 381, № 2, 173, (2002)