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Review/Research article/Short communication https://doi.org/10.17308/kcmf.2025.27/000

Modelling of interdiffusion and phase formation in thin-film two-layer systems of polycrystalline oxides of titanium and cobalt

(All proper nouns should be capitalized; titles and subtitles should be left-aligned)

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Abstract

The abstract should be 200-250 words and include the following sections.

Purpose: States the problem considered in the article, its importance, and the purpose of the research.

Experimental: Provides information about the objects being studied and the methods used.

Conclusions: Provides a brief description of the principal results, major conclusions, and their scientific and practical relevance.

Keywords: Please, provide 5-10 keywords for the principal concepts, results, and terms used in the article.

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ARTICLE STRUCTURE (IMRAD)

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Single crystals of difluorides of alkaline earth elements are widely used as photonics materials [1-3] as well as matrices for doping with rare-earth ions [4,10].

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At the end of the Conclusions the authors should include notes that explain the actual contribution of each co-author to the work.

Example 1:

Nikolay N. Afonin – Scientific management, Research concept, Methodology development, Writing – original draft, Final conclusions.

Vera A. Logachova – Investigation, Writing – review & editing.

Example 2:

The authors contributed equally to this article.

Conflict of interests

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

References

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- 1. Bahadur A., Hussain W., Iqbal S., Ullah F., Shoaib M., Liu G., Feng K. A morphology controlled surface sulfurized $CoMn_2O_4$ microspike electroncatalyst for water splitting with excellent OER rate for binder-free electrocatalytic oxygen evolution. *Journal of Materials Chemistry A.* 2021;20(9): 12255–12264. https://doi.org/10.1039/D0TA09430G
- 2. Alexandrov A. A., Mayakova M. N., Voronov V. V., Pominova D. V., Kuznetsov S. V., Baranchikov A. E., Ivanov V. K., Fedorov P. P. Synthesis upconversion luminophores based on calcium fluoride. *Condensed Matter and Interphases*. 2020;22(1): 3–10. https://doi.org/10.17308/kcmf.2020.22/2524
- 3. Kopeychenko E. I., Mittova I. Y., Perov N. S., Alekhina Y. A., Nguyen A. T., Mittova V. O., Pham V. Synthesis, composition and magnetic properties of cadmium-doped lanthanum ferrite nanopowders. *Inorganic Materials*. 2021;57(4): 367–371. https://doi.org/10.1134/S0020168521040075

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- 4. Nakamoto K. *Infrared and Raman spectra of inorganic and coordination compounds*. New York: John Wiley; 1986. 479 p.
- 5. Fedorov P. P., Osiko V. V. Crystal growth of fluorides. In: *Bulk Crystal Growth of Electronic. Optical and Optoelectronic Materials*. P. Capper (ed.). Wiley Series in Materials for Electronic and Optoelectronic Applications. John Wiley & Son. Ltd.; 2005. pp. 339-356. https://doi.org/10.1002/9780470012086.ch11
- 6. *Nanostructured oxide materials in modern micro-, nano- and optoelectronics*. V. A. Moshnikov, O. A. Aleksandrova (eds.). Saint Petersburg: Izd-vo SPbGETU "LETI" Publ., 2017. 266 p. (in Russ.)

Conference proceeding: individual paper

7. Afonin N. N., Logacheva V. A., Khoviv A. M. Synthesis and properties of functional nanocrystalline thin-film systems based on complex iron and titanium oxides. In: *Amorphous and microcrystalline semiconductors: Proc. 9th Int. Conf.*, 7–10 July 2014. St. Petersburg: Polytechnic University Publ.; 2014. p. 356–357. (In Russ.)

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Website

8. NIST Standard Reference Database 71. *NIST Electron Inelastic-Mean-Free-Path Database: Version 1.2.* Available at: www.nist.gov/srd/nist-standard-reference-database-71

Patent

9. Chekanov V. V., Kandaurova N. V., Rakhmanina Yu. A., Chekanov V. S. *Ultrasound indicator 2*. Patent RF, no. 2446384, 2012. Publ. 27.03.2012, bull. no. 9. (In Russ.)

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Example:

- **Fig. 1.** Dependences of the parameters a and c of the tetragonal lattice of nanocrystalline PdO films on the oxidation temperature T_{ox} : 1 single-phase PdO films, 2 heterophase PdO + Pd films; 3 data of the ASTM standard [22, 23]
- **Table 1.** The values of relative electronegativity (ENE) of some chemical elements [30] and the proportion of the ionic component of the chemical bond in binary compounds of the AB composition formed by these elements

1100

1200

1000

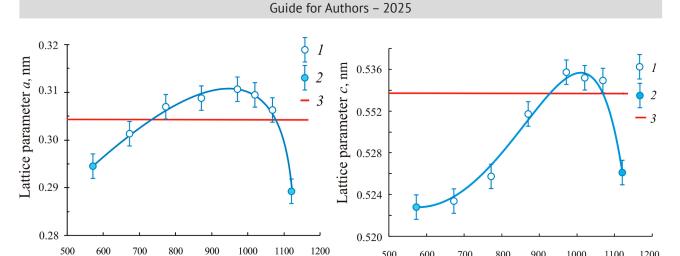


Fig. 1. Dependences of the parameters *a* and *c* of the tetragonal lattice of nanocrystalline PdO films on the oxidation temperature T_{ox} : 1 – single-phase PdO films; 2 – heterophase PdO + Pd films; 3 – data of the ASTM standard [22, 23]

500

600

700

800

Oxidation temperature T_{ox} , K

900

1200

Table 1. Values of the ionic radii of palladium Pd²⁺ and oxygen O²⁻ [30–32]

1100

Ion	Coordination number CN	Coordination polyhedron	Values of ionic radii $R_{\rm ion}$, nm
Pd^{2+}	4	Square (rectangular)	0.078 [30]; 0.086 [31]; 0.078 [32]
O ²⁻	4	Tetragonal tetrahedron	0.132 [30]; 0.140 [31]; 0.124* [31]; 0.132 [32]

^{*}The values of ionic radius were obtained on the basis of quantum mechanical calculations.

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