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Review/Original article/Short communication
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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)

N. N. Afonin^{*1}, V.A. Logacheva²

¹Voronezh State Pedagogical University,
86 ul. Lenina, Voronezh 394043, Russian Federation
(Official name and address of the organisation)

²Voronezh State University,
1 Universitetskaya pl., Voronezh 394018, Russian Federation

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.

Acknowledgements: Please, list the organisations that provided the funding for the research.

Example: the work was carried out within the framework of project No... supported by the Russian Science Foundation. The authors are grateful to PhD in Chemistry V. S. Semeykina (Siberian Branch of the Russian Academy of Sciences) for help ...

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*Nikolay N. Afonin, nafonin@vspu.ac

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Article structure

The main text of the manuscript should have the following structure.

1. Introduction

The introduction (1–2 pages) states the problem under consideration, its relevance, and the most important tasks that need to be resolved. Describe the scientific problems which have not yet been solved and which you sought to solve in your research. The introduction should contain a short critical review of previously published works in this field and their comparative analysis. It is recommended that the analysis is based on 20–30 studies. **The purpose** of the article is indicated by the problem statement.

The Vancouver reference style is used in the journal: bibliographic references in the text of the article are indicated by numbers in square brackets; in the references section, the references are numbered in the order they are mentioned in the text.

Example of references in-text citations:

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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The experimental section (2–3 pages) provides the details of the experiment, the methods, and the equipment used. The object of the study and the stages of the experiment are described in detail and the choice of research methods is explained.

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Example:

1.1. X-ray diffraction analysis

Example of figure captions in the text of the article: Fig. 1, curve 1, Fig. 2b.

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4. Conclusions

Conclusions (1 paragraph) should briefly state the main conclusions of the research. Do not repeat the text of the article. The obtained results are to be considered with respect to the purpose of the research. This section includes the conclusions, a summary of the results, and recommendations. It states the practical value of the research and outlines further research problems in the corresponding field.

Contribution of the authors

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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Examples:

Articles in scientific journals

1. Luo Y., Zhao J. Plasmon-exciton interaction in colloiddally fabricated metal nanoparticle-quantum emitter nanostructures. *Nano Research*. 2019;12(9): 2164–2171. <https://doi.org/10.1007/s12274-019-2390-z>

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. *Kondensirovannye sredy i mezhfaznye granitsy = Condensed Matter and Interphases*. 2020;22(1): 3–10. <https://doi.org/10.17308/kcmf.2020.22/2524>

3. Ryabtsev S. V., Shaposhnik A. V., Samoylov A. M., Sinelnikov A. A., Soldatenko S. A., Kushchev S. B., Ievlev V. M. Thin films of palladium oxide for gas sensors. *Doklady Physical Chemistry*. 2016;470(2): 158–161. <https://doi.org/10.1134/s0012501616100055>

Books: print

4. Kofstad P. *Nonstoichiometry, diffusion, and electrical conductivity in binary metal oxides*. Wiley-Interscience; 1972. 382 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>

References to online sources

6. 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

Conference proceedings: individual papers

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.)

Information about the authors

This section should include the full last and first name(s) of the author(s), their academic degree, academic title, affiliation, position, city, country, e-mail, and ORCID (register for an ORCID here <https://orcid.org/register>).

Example:

Nikolay N. Afonin, DSc in Chemistry, Research Fellow, Professor at the Department of *Science and Technology Studies*, Voronezh State Pedagogical University, Voronezh, Russian Federation; e-mail: nafonin@vspu.ac.ru. ORCID iD: <https://orcid.org/0000-0002-9163-744X>.

Vera A. Logachova, PhD in Chemistry, Research Fellow at the Department of General and Inorganic Chemistry, Voronezh State University, Voronezh, Russian Federation; e-mail: kcmf@main.vsu.ru. ORCID iD: <https://orcid.org/0000-0002-2296-8069>.

Valery V. Voronov, PhD in Physics and Mathematics, Head of the Laboratory, Prokhorov General Physics Institute of the Russian Academy of Science, Moscow, Russian Federation; e-mail: voronov@lst.gpi.ru. ORCID iD: <https://orcid.org/0000-0001-5029-8560>.

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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

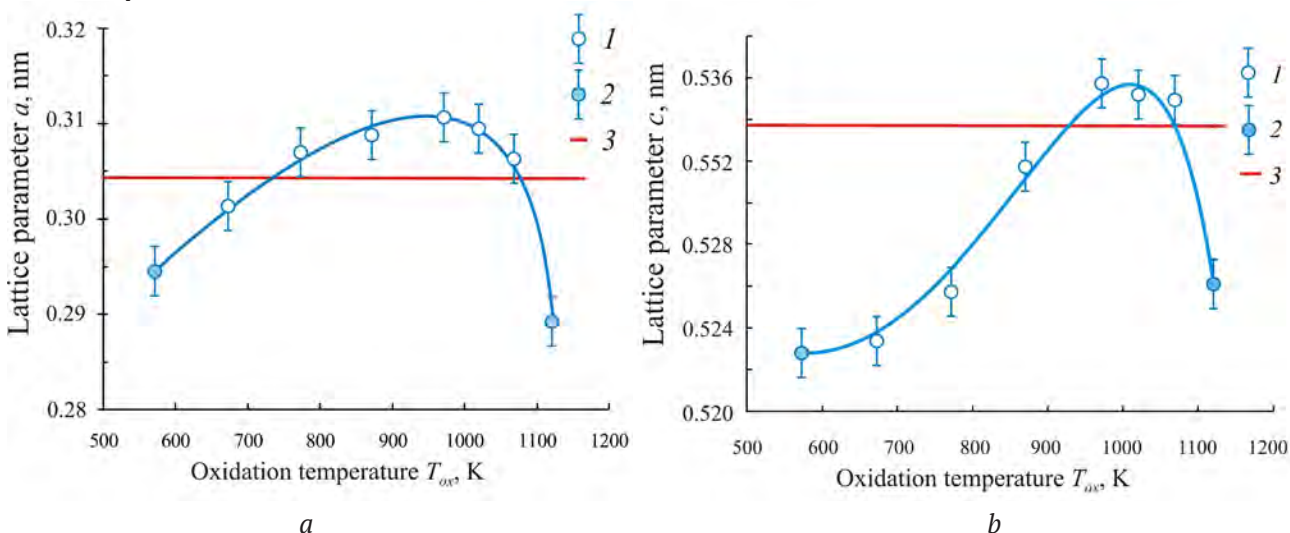


Fig. 1. Dependences of the parameters a and c of the tetragonal lattice of nanocrystalline PdO films on the oxidation temperature T_{ox} : 1 – single-phase PdO films; 2 – heterophase PdO + Pd films; 3 – data of the ASTM standard [22, 23]

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

Ion	Coordination number CN	Coordination polyhedron	Values of ionic radii R_{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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