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Employment and positions

Institute of Metallurgy and Materials Science, Polish Academy of Sciences: assistant professor (from 10.2017 - 11.2023)

University of Warsaw Biological and Chemical Research Centre: assistant professor (since 2020-2022)

Institute of Metallurgy and Materials Science, Polish Academy of Sciences: associate professor (from 12.2023 - present)

Scientific career

M.Sc.: Jagiellonian University, Faculty of Chemistry, 2010

Ph.D.: Institute of Metallurgy and Materials Science PAS, 2015

Habilitation: Institute of Metallurgy and Materials Science PAS, 2023

Scientific achievements

ORCID: https://orcid.org/0000-0003-4802-9200

The most relevant publications during last 5 years

1.
1.

Marcela E. Trybula, Przemysław W. Szafrański and Pavel A. Korzhavyi „Structure and chemistry of liquid Al-Cu alloys: molecular dynamics study versus thermodynamics-based modelling", J. Mater. Sci., 11 (2018) 8285-8301.

2.

Marcela E. Trybula, Sylwia Terlicka, Przemyslaw Fima "Thermodynamics of liquid Li-Sb alloys - Experiment vs modeling" J. Chem. Therm., 128 (2019) 134-140.

3.

Patryk Kasza, **Marcela E. Trybula**, Katarzyna Baradziej, Przemysław W. Szafrański, Marek Cegła. „Fluorescent triazolyl spirooxazolidines: Synthesis and NMR stereochemical studies"

J. Mol. Str., 1183 (2019) 157-167.

4.

Marcela E. Trybula and Pavel A. Korzhavyi „ Atomistic Simulations of Al(100) and Al(111) Surface Oxidation: Chemical and Topological Aspects of the Oxide Structure", J. Phys. Chem. C, 123, 1, (2019) 334-346.

5.

P.W. Szafrański, **M.E. Trybula**, P. Kasza, M.T. Cegła, "Following the oxidation state of organosulfur compounds with NMR: Experimental data versus DFT calculations and database-powered NMR prediction" J. Mol. Str., 1202 (2020) 157-167.

6.

Aleksandra Drewienkiewicz, Arkadiusz Żydek, **Marcela E. Trybula** and Janusz Pstruś „Atomic Level Insight into Wetting and Structure of Ag Droplet on Graphene Coated Copper Substrate-Molecular Dynamics versus Experiment", Nanomaterials, 11(6), 2021, 1465, 1465: 1-16.

7.

Arkadiusz Żydek, Mariusz Wermiński and **Marcela E. Trybula** „ Description of grain boundary structure and topology in nanocrystalline aluminum using Voronoi analysis and order parameter" Computational Materials Science, Volume 197, (2021) 110660:1-12.

8.

Marcela E. Trybula and Pavel A. Korzhavyi „ Atomistic Simulations of Al(100) and Al(111) Surface Oxidation: Chemical and Topological Aspects of the Oxide Structure", Journal of Physical Chemistry C, 123, 1, (2019) 334-346.

9.

Marcela E. Trybula and Pavel A. Korzhavyi „Temperature dependency of structure and order evolution in 2D confined oxide films grown on Al substrates using reactive molecular dynamics", Vacuum, 190, (2021) 110243:1-8.

10.

Marcela E. Trybula, Arkadiusz Żydek, Pavel Korzhavyi, Joanna Wojewoda-Budka "Structure and behaviour of oxide-coated aluminum surface in contact with strongly alkaline and acidic aqueous solutions - a reactive molecular dynamics simulation study" Journal of Physical Chemistry C, 127 (5), (2023), 2493-2507

Research Projects

NSC Projects

-

*Thermodynamic and physical properties of liquid binary alloy*s, PRELUDIUM, 2011/03/N/ST8/05308 - principal investigator (08.2012-08.2014)

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Thermodynamic, structural and physicochemical properties of liquid Al.-Li-Zn alloys, ETIUDA, 2014/12/T/ST8/00089 - principal investigator (10.2014- 06.2015)

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Mechanism of the discontinuous precipitation reaction - an atomistic simulation study, SONATA,

NCN2016/21/D/ST8/01689 - principal investigator (10.2017-10.3019)

-

Thermodynamic and structural properties of liquid Ag-Li-Sb alloys, OPUS, NCN2015/19/B/ST8/0107 - investigator (07.2016 - 09.2017)

-

Mass transport processes in phase transformations at moving boundaries of discontinuous precipitates-experiment vs. modelling, OPUS, 2017/25/B/ST8/02198 - investigator (03.2020-12.2020)

European Union and other Projects

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Innovative and affordable service for the Preventive Conservation monitoring of individual Cultural Artefacts during display, storage, handling and transport, CollectionCare project, Horizon2020, 501-D31260-0534653 - investigator, (03.2020-01.2022)

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ALUminium oXides for processing and products, ALUX, Swedish Foundation for Strategic Research (SSF), RMA11-0090 - investigator, (01.2017-12.2018)

Experience gained abroad

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Institute of Technology in Grenoble, Grenoble, France, 2014-2015 (4 months)

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Physical Properties of Materials, Research with Neutrons and Muons Division, Paul Scherrer Institute, Villigen, Switzerland, 2015 (1 week)

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School of Chemical Technology, Aalto University, Aalto, Finland, 2015 (1 week)

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KTH Royal Institute of Technology, Stockholm, Sweden, 2017-2018 (24 months)

Prizes and awards

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2014 ETIUDA Doctoral scholarship

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2015 Larry Kauffman Scholarship

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2017 Carl Tryggers Stiftelse for Vetenskapling

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2018 Carl Tryggers Stiftelse for Vetenskapling

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2020 - 3 year fellowship for outstanding young scientists granted by Ministry of Science and Higher Education

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7.07.2015 invited seminar, Condensed Matter Theory Group at PSI, Villigen, Switzerland, entitled: "Multiscale Description of structural and thermophysical properties of liquid alloys"

Education of scientific staff

Supervisor of Master thesis: Arkadiusz Żydek, University of Technology AGH, 2020, "Impact of Grain Boundary Complexion on structural properties in aluminum alloy"

Co-supervisor of PhD thesis: Monika Bugajska Institute of Metallurgy and Materials Science, PAS, 2020, "Thermodynamic properties of liquid Ag-Li-Sb alloys"

Supervisor of internshipers:

Students from Jagiellonian University and University of Technology AGH, 2017-2019

3-months internships of ERASMUS+ student at KTH Royal Institute of Technology, Sweden, 2017

International cooperation

Department of Materials Science and Engineering, KTH Royal Institute of Technology, Stockholm, Sweden - Prof. Pavel Korzhavyi

Organisation of conferences and scientific events

Co-organizator of discussion panel M8: Predicting Interface Structure and Dynamics - From Atomic- to Meso-Scale Materials Science and Engineering Congress (MSE) Darmstadt, Germany, 25.09-27.09.2018

Co-organizator of discussion panel M16: Predicting Interface Structure and Dynamics - From Atomic- to Meso-Scale Materials Science and Engineering Congress (MSE) Darmstadt, Germany, 22.09.- 25.09.2020

Co-organizator of discussion panel M01: Interfaces in Advanced Materials: From Atomistic - to Meso-Scale Materials Science and Engineering Congress (MSE) Darmstadt, Germany, 27.09.-29.09.2022

Membership in professional societies

TMS since 2014

Member of Discussion Panel of Crystals MDPI, 2020

Main areas of scientific interests

Structure and properties of liquid aluminum based alloys, thin films and grain boundary studies of manocrystalline and polycrystalline aluminum and its alloys at the nanoscale, computational materials science (molecular dynamics, Monte Carlo, DFT calculations, Voronoi polyhedral analysis), semi-empirical modelling