ROBERT J. PARUCH, PH.D.

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SUMMARY

Computational physicist interested in computer modeling of physical phenomena, associated analytical tools software development and data analysis aimed at improving the efficiency and productivity of experimental setups. Over nine years of experience in academic research on modeling of sputtering of materials by energetic particles and building analytical models to interpret the results of simulations. Coauthored over 25 scientific publications as a result of independent and collaborative work within the research group. Looking for an opportunity of transition to the industrial workplace leveraging the gained experience and developed skills, aligned with professional interests and ensuring motivating and supportive work environment with encouraging career prospects.

KEY SKILLS AND EXPERIENCE

- Developing computer codes and algorithms to support the research in materials modeling of atomic and molecular solids (differential equations, statistical analysis)
- Scientific scripting, programming and code optimization (Python, C/C++, Fortran, Tcl, Java)
- Processing, analysis and graphical visualization of very large datasets such as molecular dynamics trajectories (automation scripting)
- Simulation techniques (Molecular Dynamics, Monte Carlo)
- Numerical methods (linear algebra, ODEs, PDEs), graphing and analytic packages (matplotlib, PyLab, Gnuplot, Origin Pro, Mathematica), molecular modeling and visualization programs (Visual Molecular Dynamics, Materials Studio)
- Scientific writing, peer reviewing, document formatting, and presenting the results of research at conferences and workshops (MS Office, LaTeX, Adobe Photoshop)
- Familiarity with software development practices (IDE's, version control, debugging), and querying a database (SQL)
- Familiarity with parallel and distributed computing practices using remote HPC clusters (Bash, SSH, PBS)
- Familiarity with operating systems (Windows, Linux, Android), networking (IP) and computer architecture (PC assembly)

WORK EXPERIENCE

THE PENNSYLVANIA STATE UNIVERSITY, UNIVERSITY PARK, PA — 2012 – 2017

Postdoctoral Scholar, Department of Chemistry

- Conducted research on sputtering and depth profiling of molecular solids. The protocol included performing molecular dynamics simulations of multiple-cluster irradiation of molecular solids and interpretation of the results with an analytical model, previously developed and then improved, the Steady-State Statistical Sputtering Model. The most important achievement was the calculation of a depth profile of the molecular solid utilizing the developed novel method. Such a result, derived from an entirely computational procedure, had never been reported in the literature before. The obtained results facilitated association of the beam conditions and material properties of molecular solids with the depth profile characteristics, which is of important experimental interest in order to improve the accuracy and specificity of the Secondary-Ion Mass Spectrometry analytical technique
- Demonstrated that the universal concept in sputtering yields has a physical basis based on similarities in ejection mechanisms between molecular and atomic solids. The obtained results provided a new understanding of the experimental findings reported in the literature
- As part of a collaborative work, coded the macroscopic transport model based on the advection-diffusion-reaction equation in Python. Demonstrated that this approach is applicable to modeling of depth profiling for larger time and length scales that are directly comparable with the experimental quantities, which laid the groundwork for further model approaches to interpret the results of depth profiling simulations
- This work resulted in 10 research papers published in peer-review journals and international conferences, including six papers coauthored as the first author. Presented the research results at four international conferences

JAGIELLONIAN UNIVERSITY, KRAKOW, POLAND — 2008 – 2012

Graduate Research Assistant, Department of Nanostructures and Nanotechnology

- Conducted research on depth profiling of atomic solids. The protocol included performing molecular dynamics simulations of multiple-cluster irradiation of metal samples and interpretation of the results with a newly developed analytical model, the Steady-State Statistical Sputtering Model. The developed novel method provided insight into the dynamics of irradiation induced processes

in atomic solids (surface topography development, ion-beam mixing) and facilitated an explanation of the dependence of depth profile properties on the beam conditions, which is of important experimental interest
- This work resulted in nine research papers published in peer-review journals and international conferences, including three papers coauthored as the first author. Presented the research results at three international conferences

THE PENNSYLVANIA STATE UNIVERSITY, UNIVERSITY PARK, PA — 2011

Visiting Scholar, Department of Chemistry

- Solely responsible for coding the Steady-State Statistical Sputtering Model in Python, utilizing the PyLab package. Performed molecular dynamics simulations of multiple-impact cluster irradiation of metal samples on the remote computing cluster at the Penn State HPC center. This work was a part of the research projects described above

JAGIELLONIAN UNIVERSITY, KRAKOW, POLAND — 2006 – 2008

Undergraduate Research Assistant, Department of Nanostructures and Nanotechnology

- Conducted research on sputtering of Langmuir-Blodgett multilayers. The protocol included designing a coarse-grained computer model of a Langmuir-Blodgett multilayer composed of bariated arachidic acid molecules and performing molecular dynamics simulations of single-cluster irradiation of aforementioned systems. The obtained results of simulations facilitated an explanation of the anisotropic effects observed experimentally and were published in two peer-review research papers

SELECTED RESEARCH PUBLICATIONS

- D. Maciazek, **R. J. Paruch**, Z. Postawa, and B. J. Garrison, *Micro- and Macroscopic Modeling of Depth Profiling*, J. Phys. Chem. C 120: 25473-25480, 2016
- **R. J. Paruch**, Z. Postawa, and B. J. Garrison, *Seduction of Finding Universality in Sputtering Yields Due to Cluster Bombardment of Solids*, Acc. Chem. Res. 48: 2529-2536, 2015
- **R. J. Paruch**, B. J. Garrison, M. Mlynek, and Z. Postawa, *On Universality in Sputtering Yields Due to Cluster Bombardment*, J. Phys. Chem. Lett. 5: 3227-3230, 2014
- **R. J. Paruch**, B. J. Garrison, and Z. Postawa, *Computed Molecular Depth Profile for C_{60} Bombardment of a Molecular solid*, Anal. Chem. 85: 11628-11633, 2013
- **R. J. Paruch**, B. J. Garrison, and Z. Postawa, *Partnering analytic models and dynamic secondary ion mass spectrometry simulations to interpret depth profiles due to kiloelectronvolt cluster bombardment*, Anal. Chem. 84: 3010-3016, 2012
- **R. J. Paruch**, Z. Postawa, A. Wucher, and B. J. Garrison, *Steady-State Statistical Sputtering Model for Extracting Depth Profiles from Molecular Dynamics Simulations of Dynamic SIMS*, J. Phys. Chem. C 116: 1042-1051, 2012
- **R. Paruch**, L. Rzeznik, M. F. Russo, B. J. Garrison, and 2Z. Postawa, *Molecular Dynamics Study of the Effect of Surface Topography on Sputtering Induced by 20 keV Au_3 and C_{60} Clusters*, J. Phys. Chem. C 114: 5532-5539, 2010
- **R. Paruch**, L. Rzeznik, B. Czerwinski, B. J. Garrison, N. Winograd, and Z. Postawa, *Molecular dynamics simulations of sputtering of Langmuir-Blodgett multilayers by keV C_{60} projectiles*, J. Phys. Chem. C 113: 5641-5648, 2009

SELECTED CONFERENCE PRESENTATIONS

- **R. J. Paruch**, Z. Postawa, and B. J. Garrison, *Exploration of the concept of universality in sputtering yields due to cluster bombardment*, 20th International Conference on Secondary Ion Mass Spectrometry, Seattle, WA, September 13-18, 2015
- **R. J. Paruch**, Z. Postawa, and B. J. Garrison, *How material properties affect depth profiles – insight from computer modeling*, 19th International Conference on Secondary Ion Mass Spectrometry, Jeju, Korea, September 29-October 4, 2013
- **R. Paruch**, B. J. Garrison, and Z. Postawa, *Extraction of Depth Profiles from Steady-state MD Simulations of C_{60}/Ag(111) repetitive bombardment*, 18th International Conference on Secondary Ion Mass Spectrometry, Riva del Garda, Italy, September 18-23, 2011

EDUCATION

JAGIELLONIAN UNIVERSITY, KRAKOW, POLAND — 2012

Doctor of Philosophy in Physics

- Dissertation: *Computer modeling of depth profiling of crystal samples with C_{60} and Au_3 cluster projectile beams*

JAGIELLONIAN UNIVERSITY, KRAKOW, POLAND — 2008

Master of Science in Physics, majoring in Computational Physics

- Thesis: *Computer modeling of sputtering of arachidic acid films by C_{60} cluster projectiles*