Maksim S. Rakitin

Bio

Personal details

Name: Maksim S. Rakitin

Summary: I am a computational scientist at NSLS-II, BNL. I help beamline staff and users run scientific experiments and perform data analysis. I write code in Python to integrate hardware (motors, cameras, detectors, *etc.*) and 3rd-party software systems with the Bluesky data acquisition framework. I am developing the Sirepo-Bluesky library that integrates Bluesky and the Sirepo browser-based interface to scientific modeling codes to enable access to "virtual" beamlines. I am a proponent of well-tested, modular, reusable, sustainable, and easily accessible code. I am fluent with modern CI systems (GitHub Actions, MS Azure Pipelines, *etc.*) I use Docker/Podman (including the creation of images), Linux (RHEL8, CentOS, Ubuntu, *etc.*), vagrant/VirtualBox on a daily basis. I am maintaining over 100 conda-forge feedstocks (Python, Python with C-extensions, C/C++, Fortran). I lead the continuous integration efforts to deploy and test the conda environments with the Bluesky software stack. I am enthusiastic about new technologies and AI/ML projects. I am a PI on an AI/ML LDRD project and a PI for two SBIR subcontracts with Radiasoft LLC (total funds of $1M+).

News: "Computer, Is My Experiment Finished?" (September 16, 2022)
https://www.bnl.gov/newsroom/news.php?a=220832

"Seeing the Forest Through the Trees: Brookhaven Lab Scientists Develop New Computational Approach to Reduce Noise in X-ray Data." (April 18, 2022)
https://www.bnl.gov/newsroom/news.php?a=219533

Links:
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Education and training

2008.10–2012.09 **Ph.D. in Condensed Matter Physics (defended on September 19, 2012)**
South Ural State University (National Research University), Chelyabinsk, Russia

2006.09–2008.06 **M.S. in Applied Mathematics and Physics (June 13, 2008)**
South Ural State University (SUSU), Chelyabinsk, Russia

2002.09–2006.06 **B.S. in Applied Mathematics and Physics (June 20, 2006), summa cum laude**
South Ural State University (SUSU), Chelyabinsk, Russia

Research and professional expertise

2017.11–present **Associate Computational Scientist**, *DAMA group, NSLS-II, Brookhaven National Laboratory*, Upton, NY (https://www.bnl.gov)

2015.12–2017.10 **Research Associate (Postdoc)**, *NSLS-II, Brookhaven National Laboratory*, Upton, NY (https://www.bnl.gov)

2013.10–2015.12 **Postdoctoral Associate (Postdoc)**, *Department of Geosciences, Stony Brook University*, Stony Brook, NY (https://stonybrook.edu, https://uspex-team.org/en)

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2007.06–2013.10 **QA Engineer, QA Team Leader**, *Applied Technologies Ltd.*, Chelyabinsk, Russia (http://www.appliedtech.ru), a partner of Rocket Software Inc., USA (https://www.rocketsoftware.com)

Software projects

- **Bluesky** — a library for experiment control and collection of scientific data and metadata, https://blueskyproject.io/bluesky.
- **Ophyd** — a device abstraction library, https://blueskyproject.io/ophyd.
- **Databroker** — a simple, user-friendly interface for retrieving stored data and metadata from multiple sources, https://blueskyproject.io/databroker.
- **Synchrotron Radiation Workshop (SRW)** — computer code for X-ray source and optics simulations, https://github.com/mrakitin/SRW.
- **Sirepo** — a cloud-based framework for SRW, https://github.com/radiasoft/sirepo.
- **Databroker extractor** — image processing and data visualization, https://github.com/mrakitin/databroker-extractor.
- **CRL simulator** — a code for simulation of a transfocator (compound refractive lenses (CRL) for X-ray focusing), https://github.com/mrakitin/bnlcrl.
- **USPEX** — a code for evolutionary crystal structure prediction, https://uspex-team.org/en.
- **USPEX online utilities** — a set of pre- and post-processing tools for crystal structure simulations, http://han.ess.sunysb.edu.
- **USPEX manual** — http://han.ess.sunysb.edu/uspex_manual.
- Utilities for DFT simulations
- IBM Mainframe software projects

Publications

41. T. W. Morris, M. Rakitin, A. Giles, J. Lynch, A. L. Walter, B. Nash, D. Abell, P. Moeller, I. Pogorelov, and N. Goldring, "On-the-fly optimization of synchrotron beamlines using machine learning," in *Optical System Alignment, Tolerancing, and Verification XIV*, J. Sasián and R. N. Youngworth, Eds., vol. 12222, International Society for Optics and Photonics. SPIE, 2022, p. 122220M. https://doi.org/10.1117/12.2644996
40. T. Konstantinova, L. Wiegart, M. Rakitin, A. M. DeGennaro, and A. M. Barbour, "Machine Learning for analysis of speckle dynamics: quantification and outlier detection," *Phys. Rev. Research*, vol. 4, p. 033228, Sep. 2022. https://link.aps.org/doi/10.1103/PhysRevResearch.4.033228
39. D. Leshchev, M. Rakitin, B. Luvizotto, R. Kadyrov, B. Ravel, K. Attenkofer, and E. Stavitski, "The Inner Shell Spectroscopy beamline at NSLS-II: a facility for in situ and operando X-ray absorption spectroscopy for materials research," *Journal of Synchrotron Radiation*, vol. 29, no. 4, Jul. 2022. https://doi.org/10.1107/S160057752200460X
38. D. Hidas, A. M. Kiss, M. Rakitin, J. Sinsheimer, T. Tanabe, and M. Musardo, "High precision real-time insertion device and monochromator synchronization at NSLS-II," *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, vol. 1031, p. 166505, Mar. 2022. https://doi.org/10.1016/j.nima.2022.166505
37. B. Nash, D. T. Abell, D. L. Bruhwiler, E. G. Carlin, Y. Du, J. P. Edelen, A. Giles, M. V. Keilman, J. Lynch, J. Maldonado, P. Moeller, R. Nagler, I. V. Pogorelov, M. S. Rakitin, A. Walter, and S. D. Webb, "X-Ray Beamline Control with Machine Learning and an Online Model," in *Proc. ICALEPCS'21*, ser. International Conference on Accelerator and Large Experimental Physics Control Systems, no. 18. JACoW Publishing, Geneva, Switzerland, Dec. 2021, pp. 695–699. https://doi.org/10.18429/JACoW-ICALEPCS2021-WEPV024
36. R. Jain, D. Abel, M. Rakitin, M. Sullivan, D. T. Lodowski, M. R. Chance, and E. R. Farquhar, "New high-throughput endstation to accelerate the experimental optimization pipeline for synchrotron X-ray footprinting," *Journal of Synchrotron Radiation*, vol. 28, no. 5, pp. 1321–1332, Sep. 2021. https://doi.org/10.1107/S1600577521005026
35. L. Yang, E. Lazo, J. Byrnes, S. Chodankar, S. Antonelli, and M. Rakitin, "Tools for supporting solution scattering during the COVID-19 pandemic," *Journal of Synchrotron Radiation*, vol. 28, no. 4, pp. 1237–1244, Jul. 2021. https://doi.org/10.1107/S160057752100521X
34. M. S. Rakitin and A. A. Mirzoev, "Ab initio Simulation of Dissolution Energy and Bond Energy of Hydrogen with 3sp, 3d, and 4d Impurities in bcc Iron," *Phys. Solid State*, vol. 63, no. 7, pp. 1065–1068, Jul. 2021. https://doi.org/10.1134/S1063783421070180
33. T. Konstantinova, L. Wiegart, M. Rakitin, A. M. DeGennaro, and A. M. Barbour, "Noise reduction in X-ray photon correlation spectroscopy with convolutional neural networks encoder–decoder models," *Sci Rep*, vol. 11, no. 1, Jul. 2021. https://doi.org/10.1038/s41598-021-93747-y

32. S. I. Campbell, D. B. Allan, A. M. Barbour, D. Olds, M. S. Rakitin, R. Smith, and S. B. Wilkins, "Outlook for artificial intelligence and machine learning at the NSLS-II," *Machine Learning: Science and Technology*, vol. 2, no. 1, p. 013001, Mar. 2021. https://doi.org/10.1088/2632-2153/abbd4e

31. O. Chubar, L. Wiegart, S. Antipov, R. Celestre, R. Coles, A. Fluerasu, and M. Rakitin, "Analysis of hard x-ray focusing by 2D diamond CRL," in *Advances in Computational Methods for X-Ray Optics V*, O. Chubar and K. Sawhney, Eds., vol. 11493, International Society for Optics and Photonics. SPIE, Aug. 2020, pp. 119–127. https://doi.org/10.1117/12.2568980

30. O. Chubar, R. A. Coles, L. Wiegart, A. Fluerasu, M. Rakitin, J. Condie, P. Moeller, and R. Nagler, "Simulations of coherent scattering experiments at storage ring synchrotron radiation sources in the hard x-ray range," in *Advances in Computational Methods for X-Ray Optics V*, O. Chubar and K. Sawhney, Eds., vol. 11493, International Society for Optics and Photonics. SPIE, Aug. 2020, pp. 201–208. https://doi.org/10.1117/12.2568833

29. A. He, O. Chubar, M. Rakitin, L. Samoylova, C. Fortmann-Grote, S. Yakubov, and A. Buzmakov, "Parallel performance of "Synchrotron Radiation Workshop" code: partially coherent calculations for storage rings and time-dependent calculations for XFELs," in *Advances in Computational Methods for X-Ray Optics V*, O. Chubar and K. Sawhney, Eds., vol. 11493, International Society for Optics and Photonics. SPIE, Aug. 2020, pp. 78–87. https://doi.org/10.1117/12.2567448

28. M. S. Rakitin, A. Giles, K. Swartz, J. Lynch, P. Moeller, R. Nagler, D. B. Allan, T. A. Caswell, L. Wiegart, O. Chubar, and Y. Du, "Introduction of the Sirepo-Bluesky interface and its application to the optimization problems," in *Advances in Computational Methods for X-Ray Optics V*, O. Chubar and K. Sawhney, Eds., vol. 11493, International Society for Optics and Photonics. SPIE, Aug. 2020, pp. 209–226. https://doi.org/10.1117/12.2569000

27. B. Nash, O. Chubar, D. Bruhwiler, M. Rakitin, P. Moeller, R. Nagler, and N. Goldring, "Undulator radiation brightness calculations in the Sirepo GUI for SRW," in *Advances in Laboratory-based X-Ray Sources, Optics, and Applications VII*, A. Murokh and D. Spiga, Eds., vol. 11110, International Society for Optics and Photonics. SPIE, 2019, pp. 79–92. https://doi.org/10.1117/12.2530663

26. B. Nash, N. Goldring, D. L. Bruhwiler, O. Tchoubar, A. He, M. Rakitin, R. Nagler, and P. Moeller, "Phase IIA Final Technical Report for "Development of software framework for x-Ray optics simulation and modeling"," Jul. 2019. https://www.osti.gov/biblio/1532614

25. D. Allan, T. Caswell, S. Campbell, and M. Rakitin, "Bluesky's Ahead: A Multi-Facility Collaboration for an a la Carte Software Project for Data Acquisition and Management," *Synchrotron Radiation News*, vol. 32, no. 3, pp. 19–22, 2019. https://doi.org/10.1080/08940886.2019.1608121

24. L. Wiegart, M. Rakitin, Y. Zhang, A. Fluerasu, and O. Chubar, "Towards the simulation of partially coherent x-ray scattering experiments," *AIP Conference Proceedings*, vol. 2054, no. 1, p. 060079, 2019. https://doi.org/10.1063/1.5084710

23. B. Nash, O. Chubar, N. Goldring, D. L. Bruhwiler, P. Moeller, R. Nagler, and M. Rakitin, "Detailed x-ray brightness calculations in the sirepo GUI for SRW," *AIP Conference Proceedings*, vol. 2054, no. 1, p. 060080, 2019. https://doi.org/10.1063/1.5084711

22. M. S. Rakitin, P. Moeller, R. Nagler, B. Nash, D. L. Bruhwiler, D. Smalyuk, M. Zhernenkov, and O. Chubar, "*Sirepo*: an open-source cloud-based software interface for X-ray source and optics simulations," *Journal of Synchrotron Radiation*, vol. 25, no. 6, pp. 1877–1892, Nov. 2018. https://doi.org/10.1107/S1600577518010986

21. A. Blednykh, B. Bacha, G. Bassi, W. Cheng, O. Chubar, A. Derbenev, R. Lindberg, M. Rakitin, V. Smaluk, M. Zhernenkov, Y.-c. K. Chen-Wiegart, and L. Wiegart, "New aspects of longitudinal instabilities in electron storage rings *(DOE Science Highlight)*," *Scientific Reports*, vol. 8, no. 1, p. 11918, 2018. https://doi.org/10.1038/s41598-018-30306-y

20. O. Chubar, C. Kitegi, Y.-C. K. Chen-Wiegart, D. Hidas, Y. Hidaka, T. Tanabe, G. Williams, J. Thieme, T. Caswell, M. Rakitin, L. Wiegart, A. Fluerasu, L. Yang, S. Chodankar, and M. Zhernenkov, "Spectrum-Based Alignment of In-Vacuum Undulators in a Low-Emittance Storage Ring," *Synchrotron Radiation News*, vol. 31, no. 3, pp. 4–8, 2018. https://doi.org/10.1080/08940886.2018.1460173

19. M. Rakitin, A. A. Mirzoev, and D. A. Mirzaev, "First-Principles and Thermodynamic Simulation of Elastic Stress Effect on Energy of Hydrogen Dissolution in Alpha Iron," *Russian Physics Journal*, vol. 60, no. 12, pp. 2136–2143, Apr. 2018. https://doi.org/10.1007/s11182-018-1337-2

18. M. S. Rakitin, O. Chubar, P. Moeller, R. Nagler, and D. L. Bruhwiler, "Sirepo: a web-based interface for physical optics simulations - its deployment and use at NSLS-II **(invited paper)**," in *Proc. SPIE, Advances in Computational Methods for X-Ray Optics IV (23 August 2017)*, vol. 10388, 2017, p. 103880R. https://doi.org/10.1117/12.2274031

17. O. Chubar, M. Rakitin, Y.-C. Chen-Wiegart, A. Fluerasu, and L. Wiegart, "Simulation of experiments with partially coherent x-rays using Synchrotron Radiation Workshop," in *Proc. SPIE, Advances in Computational Methods for X-Ray Optics IV (23 August 2017)*, vol. 10388, 2017, p. 1038811. https://doi.org/10.1117/12.2274481

16. O. Chubar, M. Rakitin, Y.-C. Chen-Wiegart, Y. S. Chu, A. Fluerasu, D. Hidas, and L. Wiegart, "Main functions, recent updates, and applications of Synchrotron Radiation Workshop code **(invited paper)**," in *Proc. SPIE, Advances in Computational Methods for X-Ray Optics IV (23 August 2017)*, vol. 10388, 2017, p. 1038805. https://doi.org/10.1117/12.2274285

15. L. Wiegart, M. Rakitin, A. Fluerasu, and O. Chubar, "X-ray optical simulations supporting advanced commissioning of the coherent hard x-ray beamline at NSLS-II," in *Proc. SPIE, Advances in Computational Methods for X-Ray Optics IV (23 August 2017)*, vol. 10388, 2017, p. 103880N. https://doi.org/10.1117/12.2274403

14. M. Idir, M. Rakitin, B. Gao, J. Xue, L. Huang, and O. Chubar, "Alignment of KB mirrors with at-wavelength metrology tool simulated using SRW," in *Proc. SPIE, Advances in Computational Methods for X-Ray Optics IV (23 August 2017)*, vol. 10388, 2017, p. 103880Z. https://doi.org/10.1117/12.2274264

13. M. M. Davari Esfahani, Q. Zhu, H. Dong, A. R. Oganov, S. Wang, M. S. Rakitin, and X.-F. Zhou, "Novel magnesium borides and their superconductivity," *Phys. Chem. Chem. Phys.*, vol. 19, pp. 14 486–14 494, 2017. https://doi.org/10.1039/C7CP00840F

12. O. V. Chubar, T. A. Caswell, Y. Chen-Wiegart, A. Fluerasu, Y. Hidaka, D. A. Hidas, C. A. Kitegi, M. S. Rakitin, T. Tanabe, J. Thieme, L. Wiegart, and G. Williams, "Analysis and Correction of in-Vacuum Undulator Misalignment Effects in a Storage Ring Synchrotron Radiation Source," in *Proc. of International Particle Accelerator Conference (IPAC'17), Copenhagen, Denmark, 14–19 May, 2017*, ser. International Particle Accelerator Conference, no. 8. Geneva, Switzerland: JACoW, May 2017, paper TUPAB140, pp. 1663–1665. https://doi.org/10.18429/JACoW-IPAC2017-TUPAB140

11. A. Blednykh, B. Bacha, G. Bassi, O. V. Chubar, M. S. Rakitin, V. V. Smaluk, and M. Zhernenkov, "A Comprehensive Study of the Microwave Instability," in *Proc. of International Particle Accelerator Conference (IPAC'17), Copenhagen, Denmark, 14–19 May, 2017*, ser. International Particle Accelerator Conference, no. 8. Geneva, Switzerland: JACoW, May 2017, paper WEPIK117, pp. 3224–3226. https://doi.org/10.18429/JACoW-IPAC2017-WEPIK117

10. D. A. Mirzaev, A. A. Mirzoev, and M. S. Rakitin, "Alloying Effects on Thermodynamic Characteristics of Hydrogen in BCC Iron," *Bulletin of the South Ural State University, Ser. Metallurgy*, vol. 16, no. 4, pp. 40–53, 2016, Original Russian Text. https://doi.org/10.14529/met160405

9. Y. H. R. Chang, T. L. Yoon, T. L. Lim, and M. Rakitin, "Thorough investigations of the structural and electronic properties of $Al_xIn_{1-x}N$ ternary compound via *ab initio* computations," *Journal of Alloys and Compounds*, vol. 682, pp. 338–344, 2016. https://doi.org/10.1016/j.jallcom.2016.04.281

8. M. M. Davari Esfahani, Z. Wang, A. R. Oganov, H. Dong, Q. Zhu, S. Wang, M. S. Rakitin, and X.-F. Zhou, "Superconductivity of novel tin hydrides (Sn_nH_m) under pressure," *Scientific Reports*, vol. 6, p. 22873, Mar. 2016. https://doi.org/10.1038/srep22873

7. M. S. Rakitin, A. R. Oganov, H. Niu, M. M. Davari Esfahani, X.-F. Zhou, G.-R. Qian, and V. L. Solozhenko, "A novel phase of beryllium fluoride at high pressure," *Phys. Chem. Chem. Phys.*, vol. 17, pp. 26 283–26 288, 2015. https://doi.org/10.1039/C5CP04010H

6. A. R. Oganov, C. W. Glass, A. O. Lyakhov, Q. Zhu, G.-R. Qian, H. T. Stokes, M. S. Rakitin, M. Davari, P. Bushlanov, Z. Allahyari, and S. Lepeshkin, *USPEX manual: Universal Structure Predictor: Evolutionary Xtallography*, 2013–2015. https://uspex-team.org/en/uspex/documentation

5. D. A. Mirzaev, A. A. Mirzoev, K. Y. Okishev, and M. S. Rakitin, "Theory of hydrogen solubility in binary iron alloys based on *ab initio* calculation results," *Molecular Physics*, vol. 110, no. 11-12, pp. 1299–1304, 2012. https://doi.org/10.1080/00268976.2011.645895

4. A. V. Ursaeva, M. S. Rakitin, G. E. Ruzanova, and A. A. Mirzoev, "*Ab initio* study of hydrogen interaction with point defects in bcc iron," *Bulletin of the South Ural State University: Math., Mech. and Phys.*, vol. 4, no. 10, pp. 114–119, 2011, Original Russian Text. https://vestnik.susu.ru/mmph/issue/viewFile/46/22#page=114

3. A. A. Mirzoev, D. A. Mirzaev, and M. S. Rakitin, "Impurities influence on dissolution of hydrogen in bcc iron," *Bulletin of the South Ural State University: Math., Mech. and Phys.*, vol. 4, no. 10, pp. 77–83, 2011, Original Russian Text. https://vestnik.susu.ru/mmph/issue/viewFile/46/22#page=77

2. M. S. Rakitin, A. A. Mirzoev, and D. A. Mirzaev, "Change of electronic structure in iron containing interstitial atoms of hydrogen," *Bulletin of the South Ural State University: Metallurgy*, vol. 14, no. 13, pp. 67–71, 2010, Original Russian Text. https://vestnik.susu.ru/metallurgy/issue/archive

1. A. A. Mirzoev, M. M. Yalalov, and M. S. Rakitin, "Dependence of TB-LMTO calculations accuracy on k-points number: effect of iterations mixing parameter using Broyden scheme," *Bulletin of the South Ural State University: Math., Phys. and Chem.*, vol. 6, no. 6, pp. 103–105, 2005, Original Russian Text. https://vestnik.susu.ru/mmph/issue/viewFile/36/12#page=103