Rajat Sainju, Ph.D.

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Ph.D. in Materials Science and Engineering. Over 6-plus years of extensive experience in **characterization** (in-situ gas-cell TEM, FIB, SEM, XRD, TGA) of various metals/alloys/ceramics and developing **AI/ML** (CNN, Vision-Transformers, NLP) quantitative image analysis algorithms. Problem-solver with excellent technical writing and communication skills; Co-authored 5+ peer-reviewed papers (3-first author) in leading science journals and managed 6 projects to completion.

EDUCATION

University of Connecticut Storrs, CT

Ph.D. in Materials Science and Engineering

GPA: 3.8/4.0 Aug. 2018 – June 2024

- *Relevant Coursework*: Materials Characterization, Transmission Electron Microscopy, Thermodynamics of Materials, Transport Phenomena in Materials, Structures and Defects in Materials, Machine Learning, Deep Learning, Advances in Deep Learning, Big Data Analytics
- *Dissertation*: Advancing Materials' Structural Dynamics Understanding with Deep Learning-based Quantitative Image Analysis of TEM Data.

Ramapo College of New Jersey Mahwah, NJ

Bachelor of Science in Engineering Physics; minors in Computer Science and Mathematics

GPA: 3.9/4.0 Aug. 2014 - May 2018

- *Relevant Coursework*: Photonics, Semiconductor and Optoelectronic Devices, Condensed Matter and Nuclear Physics, Quantum Mechanics I, Electrodynamics I, Experimental Methods in Physics, Data Structures, Analysis of Algorithms

PROFESSIONAL EXPERIENCE

Postdoctoral Research Associate June 2024 –

Institute of Materials Science, University of Connecticut, Storrs, CT

- Investigate the slow surface-orientation-dependent oxidation properties of tungsten (plasma-facing material in nuclear fusion reactors) in case of air ingress accidents using experimental and data analysis
- Train and mentor graduate students and postdocs on various research projects

Graduate Research Assistant Aug. 2018 – May 2024

University of Connecticut, Storrs, CT

- Conducted research on various materials: (i) heterogeneous catalysis, (ii) advanced structural alloys for nuclear fusion/fission, (iii) carbon nanotubes, and (iv) development of AI/ML image-processing algorithms for radiation defect quantification and nanoparticle phase-transition kinetic analysis
- Led graduate students for multiple research projects through training and mentoring
- Investigated and provided solutions for issues in microscopy data analysis, in-situ TEM/TGA experiments, and application of AI/ML tools encountered by the research group
- Reviewed computational and experimental data, and provided data access to project collaborators
- Presented research results at conferences and to multidisciplinary project teams from DOE-National Labs
- Assisted principal investigators in preparing proposals for securing grants in various projects and participated in research outreach activities

Major Projects:

1. **Understanding Thermal Corrosion of Plasma-facing Tungsten and the Impact of Radiation in Nuclear Fusion Extremes**

- Carried out in-situ TEM high-temperature (400°C, 500°C) corrosion studies of He-irradiated nanostructured tungsten (fuzz) that mimic LOCA and LOVA accident scenarios in nuclear fusion reactors

- Extracted first tungsten fuzz oxidation kinetic data by precise phase segmentation of TEM videos and development of robust mathematical models
- Designed novel sample transfer procedure of fuzz to MEMS e-chip (DENSsolutions) for in-situ TEM studies
- Collaborated with scientists from LANL, SNL, and UCSD, to prepare irradiated tungsten samples
- Proposed a robust multilayer-passivating oxidation mechanism in irradiated tungsten, challenging the conventional notions of the negative impact of radiation on metal oxidation
- Devised experimental workflow to investigate the slow oxidation direction of tungsten at high temperatures and identification of oxide phases using TGA, TEM, SEM, EDS/ EBSD, FIB, XRD
- Resulted in the publication of 1 peer-reviewed papers (1 in-preparation) and 2+ conference papers

2. In Situ Studies of Nanoparticle-Level Nickel Thermal Oxidation and Redispersion

- Conducted fundamental studies on thermal oxidation and optimized redox cycle redispersion of catalytic Nickel nanoparticles with broader impacts on battery, fuel cells, and catalysis
- Devised methodologies (data curation, annotation, mathematical models) to extract single particle-level oxidation (T=600C, P=2% O_2) and reduction (various T, P) kinetics by employing phase segmentation of TEM images
- Developed *NanoDetector*, modified YOLO-v5, to detect & track nanoparticle during oxidation and redox cycles
- Performed kinetic model fitting combined with microstructural evaluation to determine the dominant reaction model
- Proposed a unified oxidation theory reconciling size-dependent nickel nanoparticle oxidation
- Formulated metrics to compare and quantify redispersion yield at different pressures and temperatures
- Resulted in the publication of 1 peer-reviewed paper (1 in-preparation) and 3+ conference papers

3. Automated Quantitative Analysis of Defects in TEM Videos in Real-time

- Developed computer vision (AI/ML and non-ML) algorithms for - segmentation, detection, and tracking of irradiation defects (dislocations, loops, voids, precipitates) for high-throughput image quantification
- Established 10+ ground truth TEM datasets for a wide breadth of materials and imaging conditions
- Modified CNN architectures (U-Net, YOLOs, Mask RCNN, HRNet, CenterTrack, CenterNet, ViT) and loss functions to precisely locate and track nano-sized (20×20 pixels) irradiation defects
- Incorporated material-related evaluation metrics to enhance model training, evaluation, and performance
- Collaborated with scientists from LBNL, PNNL, ANL, and UConn CSE for project development
- Resulted in the publication of 2 peer-reviewed papers and 5+ conference papers with codes made publicly available

TECHNICAL SKILLS & LEADERSHIP EXPERIENCE

- **Laboratory Skills**: Imaging Experiments (S/TEM, in-situ E/TEM, SEM, FIB, EDS, EBSD, AFM), DENS Climate, XRD, TGA, Mechanical/Electro/Flash Polishing, NMR
- **Machine Learning/Data Analysis**: Deep Learning (CNNs, RNNs, GANs, Transformers, NLP), SVM, KNN
- **Programming**: Python (PyTorch, TensorFlow, Scikit-learn), MATLAB, C/C++, Java, SQL, HTML, Git
- **Software**: Microsoft Office (Excel, Word, PowerPoint), Origin, GIMP, LabView, Igor, ImageJ, Digital Micrograph, CaRine, Auto-CAD
- **Volunteer/Leadership**: (i) Secretary, Materials Research Society, (ii) Student Senate President, Ramapo College, (iii) Launched #StayStrongNepal social media campaign raising $8,500 to support Earthquake Victims in Nepal (iv) Raised $3,500 to provide 50 household access to solar electricity for 32 homes in rural Nepal.

PEER-REVIEWED PUBLICATIONS

1. *R. Sainju*, M. Nielsen, J. Yang, S. Suib, Y. Zhu, *In-situ ETEM Study of Nickel Nanocatalyst Regeneration Mechanisms in Redox Environments*, (*in preparation*).
2. *R. Sainju*, M. Patino, M. Baldwin, O. El Atwani, R. Kolasinski, Y. Zhu, *In-situ ETEM study of plasma-facing tungsten nanofuzz at atmospheric pressure: microstructure evolution and substrate-free kinetics*, **Acta Materialia** 278, 120282 (2024).

3. *R. Sainju*, W-Y Chen, S. Schaefer, Q. Yang, C. Ding, M. Li, Y. Zhu, *DefectTrack: a deep learning-based multi-object tracking algorithm for quantitative defect analysis of in-situ TEM videos in real-time.* **Scientific Reports** 12, 15705 (2022).
4. *R. Sainju*, D. Rathnayake, H. Tan, G. Bollas, A. M. Dongare, S. L. Suib, Y. Zhu, *In Situ Studies of Single-Nanoparticle-Level Nickel Thermal Oxidation: From Early Oxide Nucleation to Diffusion-Balanced Oxide Thickening*. **ACS Nano** 16, 6468-6479 (2022).
5. M. Togaru, *R. Sainju*, L. Zhang, W. Jiang, Y. Zhu, *Direct observation of tungsten oxidation studied by in situ environmental TEM*, **Materials Characterization** 174, 111016 (2021).
6. G. Roberts, S. Y. Haile, *R. Sainju*, D. J. Edwards, B. Hutchinson, Y. Zhu**,** *Deep Learning for Semantic Segmentation of Defects in Advanced STEM Images of Steels*. **Scientific Reports** 9, 12744 (2019).

MACHINE LEARNING MODEL DEVELOPMENT:

- Creator of *DefectTrack*: established benchmark ML dataset and built *DefectTrack,* for multi-object-tracking of defects in electron microscopy images and videos. *Featured by Argonne National Laboratory in Artificial intelligence reframes nuclear material studies*.
- Developed a novel convolutional neural network model, *DefectSegNet*, for defect segmentation in microscopic images. *Featured by DOE Energy Sciences AI Helps Scientists Quantify Irradiation Effects*.
- Detecting Gender Bias in Transformer-based Models: A Case Study on BERT https://arxiv.org/abs/2110.15733

PRESENTATIONS

1. **Microscopy and Microanalysis 2019 – 2024**. Oral Presentations.
2. UConn MSE Graduate Speaking Competition 2023.
3. UConn MSE Graduate Student Elevator Pitch Competition 2020.

HONORS AND AWARDS

- *Doctoral Dissertation Fellowship Award*, University of Connecticut, CT 2023
- *Outstanding Graduate Student Speaking Competition Award*, Department of Materials Science and Engineering, University of Connecticut, CT 2023
- *2022 Microscopy and Microanalysis Student Scholar Award*, Microscopy Society of America 2024
- *UConn Graduate School Conference Participation Award* 2021
- *Third Place, MSE Elevator Pitch Competition*, University of Connecticut, CT. 2020
- *International Spirit Award*, Ramapo College of New Jersey, NJ 2016
- *Presidential Scholar*, Ramapo College of New Jersey, NJ 2014 – 2018

Honor Societies: Alpha Sigma Mu, Sigma Pi Sigma, Alpha Lambda Delta

REFERENCES

- Yuanyuan Zhu - yuanyuan.2.zhu@uconn.edu
  Associate Professor of Materials Science and Engineering; Director, InToEM Center, UConn Tech Park, University of Connecticut
- Caiwen Ding - caiwen.ding@uconn.edu
  Associate Professor of Materials Science and Engineering, University of Minnesota
- Wei-Ying Chen – wychen@anl.gov
  Principal Materials Scientist, Nuclear Materials Group, Argonne National Laboratory