TANUJ GUPTA

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EDUCATION

Ph.D. in Mechanical Engineering, Clemson University, Clemson, SC, USA **Dec 2024**
Dissertation title: *Deformation mechanism in gold nanoparticles under compressive loading: Insights from atomistic modelling and unsupervised machine learning*
Advisor: Dr. Huijuan Zhao

M.S. in Mechanical Engineering, University of North Carolina at Charlotte, Charlotte, NC, USA **May 2019**
Thesis title: *Stress analysis of a point absorber wave energy converter*
Advisor: Dr. Alireza Tabarraei

RESEARCH EXPERIENCE

Postdoctoral Research Associate, Clemson University **Jan 2025-Present**
Multi-physics modelling of photo-acoustic non-destructive imaging:

- Developing multi-physics simulation of pulsed laser light absorption, leading to ultrasonic waves due to localized thermal expansion.
- Planning to implement a machine learning model to evaluate defects in materials.

Graduate Research Assistant, Clemson University **Aug 2019-Dec 2024**
Deformation mechanisms in gold nanoparticles using molecular dynamics:

- Developed atomistic simulation to understand the deformation mechanism of gold nanoparticles using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS).
- Leveraged machine learning techniques to identify and classify deformation mechanisms in gold nanoparticles.
- Collaborated with the experimental team at the University of South Florida and the material development team at the University of Urbana-Champaign to validate experimental work

Multi-physics simulation of a coal-fired boiler for temperature sensor installation:

- Developed a four-stage multi-physics simulation framework using ANSYS to study flue gas temperature, steam panel heat transfer, and stress distribution and support sensor design in industrial-scale boilers.
- Worked closely with interdisciplinary teams, including Advanced Material Research Lab (AMRL) and the Electric Power Research Institute (EPRI), to validate the feasibility of stainless-steel and quartz coaxial cable sensors through computational and experimental field testing, achieving 430 days of accurate temperature monitoring under extreme conditions.

Shock-induced phase transitions in fused silica using molecular dynamics:

- Applied multi-scale shock technique in LAMMPS to analyze structural changes in nano-scale fused silica under extreme strain rate.
- Investigated the influence of shock velocity to analyze the phase transition process, focusing on the nucleation, growth, and crystallinity of stishovite.

Graduate Intern, Idaho National Lab, Idaho Falls, ID, USA **May 2024-Aug 2024**

- Created finite element microstructures from experimental EBSD data of 20 tensile specimens to analyze irradiated material behavior, aiding in mechanical performance predictions.
- Developed a workflow to generate structured meshes for metamaterials using CUBIT, facilitating thermomechanical simulations.
- Gained hands-on experience simulating tritium diffusion in metal-ceramic composites .

Graduate Assistant, University of North Carolina at Charlotte (UNCC) **Jan 2018-May 2019**

- Designed and assembled a full-scale 3D multibody ocean wave energy converter model (WEC) to study dynamic structural behaviour using the commercial finite element software ABAQUS.
- Performed parametric and fatigue life analyses to predict the WEC's lifecycle and enhance its design robustness.

PATENT

PCT Patent Application: *Methods and Systems for Preparing Metal Nanostructures*, PCT/US24/41990, WO 2025/035156, filed Aug 2024. https://patents.google.com/patent/WO2025035156A1

JOURNAL PUBLICATIONS

- **Tanuj Gupta,** Micheal Wang and Huijuan Zhao, "Atomistic insights on structural transformation in gold nanoparticles ". In preparation
- **Tanuj Gupta** and Huijuan Zhao, "Machine learning assisted classification of deformation mechanism of ultrasmall gold nanoparticles ". In preparation
- **Tanuj Gupta** and Huijuan Zhao, "Shape dependent deformation in gold nanostructures ". In preparation
- **Tanuj Gupta**, Mahabubur Rahman, Xinyu Jiao, Yongji Wu, Chethan K. Acharya, Dock R. Houston, Susan Maley, Junhang Dong, Hai Xiao, and Huijuan Zhao. "Four-Stage Multi-Physics Simulations to Assist Temperature Sensor Design for Industrial-Scale Coal-Fired Boiler." Sensors, Volume 24, Issue 1, 2023.
- Md Rubayat-E Tanjil*, **Tanuj Gupta***, Matthew T. Gole*, Keegan Phayden Suero, Zhewen Yin, Donald James McCleeary, Ossie R. T. Douglas, Alissa Brooke Anderson, Catherine J. Murphy, Huijuan Zhao, Michael Cai Wang. "Nanoscale goldbeating: Solid-state transformation of 0D and 1D gold nanoparticles to anisotropic 2D morphologies." PNAS Nexus, Volume 2, Issue 8, 2023.
- Abhinav Mishra, **Tanuj Gupta**, and Bidhubhusan Sahu. "Estimation of Nuclear Separation Energy and Its Relation with Q Value." International Journal of Applied Physics and Mathematics, Volume 6, Issue 1, 2016.

CONFERENCE PROCEEDINGS

- Xinyu Jiao, Yongji Wu, Xuran Zhu, Mahabubur Rahman, **Tanuj Gupta**, D. T. Gravley, Dock Houston, Chethan. K. Acharya, Tuan Nguyen, Susan Maley, Junhung Dong, Huijuan Zhao, Hai Xiao, "Distributed Coaxial Cable Sensors for in-situ Condition Based Monitoring of Coal-Fired Boiler Tubes." International Pittsburgh Coal Conference, 2022.
- **Tanuj Gupta**, Tristan Woods, and Huijuan Zhao. "Multi-Scale Molecular Dynamics Simulation of Fused Silica Under Shock Impact: Parameter Characterizations." ASME International Mechanical Engineering Congress and Exposition(IMECE), Volume 86717, p. V009T12A035, 2022.
- **Tanuj Gupta**, Mahabubur Rahman, Chethan K. Acharya, Susan Maley, Junhang Dong, Dock R. Houston, Hai Xiao, and Huijuan Zhao. "Full Scale 3D Computational Model of the Industrial-Scale Coal Fired Boiler Performance for Temperature Sensor Installation Guidance." In ASME IMECE, Volume 85680, p. V012T12A043, 2021.

TECHNICAL PRESENTATIONS

- **Tanuj Gupta** and Huijuan Zhao. Compressing gold to the atomically thin extreme: characterization of EAM potentials, The Minerals, Metals & Materials Society (TMS) Conference March 19-23, 2024.
- **Tanuj Gupta**, Huijuan Zhao and Micheal Cai Wang, Uniaxial Compression of Spherical Gold Nanoparticles: A Molecular Dynamics Study in ASME IMECE New Orleans Oct 29th -Nov 2nd, 2023.
- **Tanuj Gupta** and Huijuan Zhao, Compress Au Nanoparticle towards 2-Dimensional Extreme: A Molecular Dynamics Study, Engineering Mechanics Institute (EMI) Conference Atlanta GA, June 6–9,

2023

- **Tanuj Gupta**, Tristan Woods, and Huijuan Zhao.” Multi-scale molecular dynamics simulation of fused silica under shock impact: parameter characterizations.” IMECE, Columbus, Ohio, Oct 2022.
- Md Rubayat-E Tanjil, **Tanuj Gupta**, Matthew Gole, Zhewen Yin, Keegan Suero, Donald McCleeary, Ossie Douglas, Alissa Anderson, Catherine Murphy, Huijuan Zhao, Michael Cai Wang, Solid-State Transformation of 0D Metal Nanoparticles to Anisotropic 2D Morphologies, Functional Nanomaterials: Functional Low-Dimensional (0D, 1D,2D) Materials, TMS Annual Meeting & Exhibition, Feb 2022.
- Xinyu Jiao, Yongji Wu, Xuran Zhu, Mahabubur Rahman, **Tanuj Gupta**, Dusting Graveley, Dock Houston, Chethan. K. Acharya, Tuan Nguyen, Susan Maley, Junhung Dong, Huijuan Zhao, Hai Xiao, Distributed Coaxial Cable Sensors for in-situ Condition Based Monitoring of Coal-Fired Boiler Tubes, International Pittsburgh Coal Conference (IPCC), PA, September 2022.
- **Tanuj Gupta**, Mahabubur Rahman, Chethan K. Acharya, Susan Maley, Junhang Dong, Dock R. Houston, Hai Xiao, and Huijuan Zhao. "Full Scale 3D Computational Model of the Industrial-Scale Coal Fired Boiler Performance for Temperature Sensor Installation Guidance." IMECE, (Online), 2021.

POSTER PRESENTATIONS/ INVITED TALKS

- **Tanuj Gupta**, The applications of molecular dynamics simulations, Mechanical Engineering Seminar, Clemson University, Aug 31st, 2023.
- **Tanuj Gupta** and Huijuan Zhao, Multi-scale molecular dynamics simulation of fused silica under shock impact, 16th Annual Materials and Optics Poster Symposium, Watt Family Innovation Center, Clemson University, May 10th, 2023.
- **Tanuj Gupta** and Huijuan Zhao, Multi-scale molecular dynamics simulation of fused silica under shock impact, Research Symposium Watt Family Innovation Center, Clemson University, Feb 27th, 2023.
- **Tanuj Gupta**, Can 2D metals be a reality? Three-Minute Thesis Presentation, Clemson University, November 11th, 2022.
- **Tanuj Gupta**, Molecular dynamics simulation of fused silica under shock impact: parameter characterizations, Graduate Seminar Research series, Mechanical Engineering, Clemson University, September 26th, 2022.

TEACHING EXPERIENCE

Graduate Lab Assistant, Clemson University **Jan 2024-Dec 2024**
Mechanical Engineering Lab II (ME 3330), Dr. Daniel Wilson

- Delivered pre-lab lectures twice a week to 2 sections of undergraduate students.
- Supervised 44 students doing lab experiments and writing professional reports.
- Evaluated lab reports and provided feedback for students to track academic progress.

Co-instructor, Clemson University **Aug 2023-Dec 2023**
Fundamentals of Atomistic Model (ME 8160), Dr. Huijuan Zhao

- Guided graduate students with a basic understanding of molecular dynamics (MD) simulations with hands-on experience running MD simulations using high-performance computing.

Graduate Grading Assistant , Clemson University **Aug 2019-Dec 2019**
Foundations of Mechanical Systems (ME3070), Dr. Pooya Niksiar

- Evaluated and assessed student performance through assignments and exams.
- Designed questions for the assignments and exams to assess and enhance students' understanding of core concepts.

Graduate Teaching Assistant, UNCC **Jan 2018-May 2019**

Mechanism (ETME 2102), Dr. Navid Gourdarzi

- Taught course material to a class of 85 students on a bi-weekly basis.
- Evaluated student performance through assignments, exams and projects.

Introduction to Computational Physics (PHYS 3210), Dr. Tino Hoffman

- Evaluated and assessed student performance through assignments, exams, and projects.
- Taught a class on coding ethics on MATLAB.

Physics tutor, Department of Physics

- Guided undergraduate students with their doubts and concepts in physics.

MENTORSHIP EXPERIENCE

Arif Sadik, Ph.D. *s*tudent **Jan 2024-Present**

- Provide guidance in conducting quality research.
- Assist with learning computational tools.

Caroline Mccoy, High school teacher **Jun 2023**

- Mentored in using atomistic simulations to study the physical behavior of particles.
- Provided training in high-performance computing applications.
- Assisted in writing MATLAB scripts for data analysis.

SERVICE TO PROFESSION

- Reviewer for ASME's IMECE **2021-Present**
- Judge for Focus on Creative Inquiry (FoCI), a university-wide forum that showcases undergraduate research at Clemson University **Apr 2023**
- Session chair for Modeling of the Fracture, Failure and Fatigue in Solids, IMECE, Columbus, OH, USA **Oct 2022**
- Judge for Undergraduate Expo poster session, IMECE, Columbus, OH, USA **Oct 2022**

HONORS AND AWARDS

- Fellowship recipient for the Computational Materials Science Summer School (CMS3), Texas A&M University **Jul 2024**
- People's choice award winner for the Science as Art competition, Clemson University **Apr 2024**
- Second place winner for Graduate Research Symposium (iGRADS) from College of Engineering, Computing, and Applied Sciences (CECAS), Clemson University **Mar 2024**
- Outstanding Graduate Student Government (GSG) Representative, Clemson University **May 2023**
- One of the candidates' winners of the Three Minute Thesis (3MT) competition from the CECAS, Clemson University **Nov 2022**
- Won election to represent the mechanical engineering department as a student senator in the Graduate Student Government, Clemson University **Aug 2022**
- Best Poster Award in Mechanical Engineering Graduate Student Poster Competition, Clemson University **Mar 2021**
- Excellent Oral Presentation Award at the 6th International Conference on Applied Physics and Mathematics (ICAPM) for the best presentation in the session, Singapore **Jan 2016**

LEADERSHIP EXPERIENCE

Senator: Graduate Student Government, Clemson University **Aug 2022-Aug 2024**

- Played a key role in organizing events, including the university-wide 3MT competition and iGRADS symposium.

Executive member: Mechanical Engineering Graduate Student Council (MEGSC), Clemson University **Aug 2022-Dec 2023**

- Conceptualized, developed, and executed the pi-MT (π-MT) Thesis Competition in the Mechanical Engineering Department, a unique adaptation of the 3MT format.

Vice-president: Nepalese Student Association (NepSA)**,** Clemson University **Aug 2022-May 2023**

- I facilitated international students from Nepal to get accustomed to Clemson and assisted with all the cultural and social events organized by the organization.

PROFESSIONAL AFFILIATION

Member: American Society of Mechanical Engineering **Aug 2021-Present**

WORKSHOPS

Artificial Intelligence for Materials Science (AIMS) Workshop, National Institute of Standards and Technology (NIST) Jul, 2023

- Explored how artificial intelligence (AI), including machine learning and deep learning, can accelerate materials discovery aligned with the Materials Genome Initiative (MGI).
- Understood the importance of diverse and curated datasets, effective material representations, inverse design, integrating theory and experiments, and choosing suitable AI algorithms.
- Gained insights into AI's potential in force-field development, generative modelling, autonomous experimentation, and even cross-disciplinary applications like natural language processing.

Advanced Materials Characterization workshop, University of Illinois Urbana-Champaign Jun 2023

- The workshop provided an overview and critical comparison of major analytical techniques for materials characterization (AFM, SEM, TEM, XRD, DSC, Raman, XPS, etc.) with an emphasis on practical applications.
- The demonstration included problem-solving strategies, instrument resolution requirements, potential data collection artefacts, and data interpretation tips.

TECHNICAL SKILLS

- Tools: LAMMPS, ANSYS, COMSOL, ABAQUS, DREAM3D, ParaView, CUBIT, MOOSE.
- Programming languages: MATLAB, Python.
- High-Performance computing (HPC): Workflow optimization, job scripting, large-scale simulations.

REFERENCES

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