Natraj Yedla

Current Position

Associate Professor
Computational Materials Engineering Group
Department of Metallurgical and Materials Engineering
National Institute of Technology Rourkela
Email: yedlan@nitrkl.ac.in; natraj9401@gmail.com
Phone: 91-6612462569 (O); 3569 (R)

Educational Qualifications

Year	Education
2013	Ph.D. (Metallurgical and Materials Engineering) Specialization: Molecular Dynamics Simulation Deformation Studies of Cu-Zr Metallic Glasses Institution: Indian Institute of Technology Kharagpur
2007	M.Tech Specialization: Industrial Metallurgy Institution: National Institute of Technology Warangal
2001	B.Tech (Metallurgical and Materials Engineering) Institution: National Institute of Technology Warangal

Research Interests

Deformation behavior and Fracture: experimental and molecular dynamics deformation studies of metals and metallic glasses.

Sponsored projects

Title:	Large-scale molecular dynamics simulation deformation studies of single crystal nickel nanowires
Sponsor:	DST-SERB
Value:	Rs 4,10,000
Duration:	January 2016- January 2019

Publications (Journals)

1) Katakam, K. C., Katakareddi, G., Mehta, K. K., & **Yedla, N**. (2023). Mechanical stability and microstructural evolution during torsion in pristine and defect nickel nanowires of different orientations: a molecular dynamics simulation study. **Molecular Simulation**, 49(8), 829-844.

2) Katakareddi, G., & **Yedla, N**. (2022). The effect of loading methods on the microstructural evolution and degree of strain localization in Cu50Zr50metallic glass composite nanowires: A molecular dynamics simulation study. **Journal of Molecular Graphics and Modelling**, 108216.

3) Katakam, K. C., & **Yedla, N.** (2022). Tensile and creep behavior of nickel nanowires containing volume defects: Insight into the deformation mechanisms and microstructural evolution using molecular dynamics simulations. **Materials Chemistry and Physics**, 277, 125560.

4) **Yedla, N.** (2021). Strain controlled fatigue response of large-scale perfect and defect nickel nanowires: A molecular dynamics study. **Journal of Molecular Graphics and Modelling**, 106, 107885.

5) Gupta, P., Majumdar, B., Katakareddi, G., & **Yedla, N**. (2021). Cu50Zr50 metallic glass flakes reinforced Al composites: Experimental and molecular dynamics nanoindentation response of matrix, interface, and reinforcement. **Journal of Non-Crystalline Solids**, 564, 120837.

6) Dora, J. K., Nayak, D., Ghosh, S., Adyam, V., **Yedla, N**., & Kundu, T. K. (2020). A facile and green synthesis approach to derive highly stable SiO x-hard carbon based nanocomposites for use as the anode in lithium-ion batteries. **Sustainable Energy & Fuels**, 4(12), 6054-6065.

7) Katakam, K. C., & **Yedla, N.** (2020). Crack velocities and microstructural investigations in nickel nanowires with crack, crack-defect under mode-I and bending using large-scale molecular dynamics simulations. **Superlattices and Microstructures**, 146, 106674.

8) Nandy, J., Sahoo, S., **Yedla, N**., & Sarangi, H. (2020). Molecular dynamics simulation of coalescence kinetics and neck growth in laser additive manufacturing of aluminum alloy nanoparticles. **Journal of molecular modeling**, 26(6).

9) Gupta, P., Katakam, K. C., Katakareddi, G., & **Yedla, N**. (2020). Crack and its interaction with defects in Al coated with Cu 50 Zr 50 metallic glass thin film: an MD simulation study. **Journal of Molecular Modeling**, 26(4), 1-17.

10) Gupta, P., Vaduganathan, K., & **Yedla, N.** (2020). Elevated Temperature Compression Behavior of Al–Cu 50 Zr 50 Nano-laminates. **Transactions of the Indian Institute of Metals**, 1-7.

11) Gupta, P., Katakam, K. C., & **Yedla, N.** (2019). High Velocity and Temperature Effects on the Bending Behavior of Nickel Nanowire: A Large-Scale Molecular Dynamics Simulation Study. **Materials Performance and Characterization**, 9(2).

12) Singh, R., Gupta, P., & **Yedla, N**. (2019). Single-crystal Al–Cu50Zr50 metallic glass cold welds: tensile and creep behaviour. **Molecular Simulation**, 45(18), 1549-1562.

13) Nandy, J., **Yedla, N**., Gupta, P., Sarangi, H., & Sahoo, S. (2019). Sintering of AlSi10Mg particles in direct metal laser sintering process: A molecular dynamics simulation study. **Materials Chemistry and Physics**, 236, 121803.

14) Dora, J. K., Sengupta, A., Ghosh, S., **Yedla, N**., & Chakraborty, J. (2019) Stress evolution with concentration-dependent compositional expansion in a silicon lithium-ion battery anode particle. **Journal of Solid State Electrochemistry**, 1-12.

15) Gupta, P., & **Yedla, N**. (2019). Tensile-compression loading and pre-strain effects on the evolution of stacking fault tetrahedra, dislocation density, and free volume in crystal-amorphous thin film interface: A large-scale molecular dynamics study. **Journal of Non-Crystalline Solids**, 514, 25-34.

16) Katakam, K. C., Gupta, P., & **Yedla, N.** (2019). Large-Scale Molecular Dynamics Simulation Studies on Deformation of Ni Nanowires: Surface Profile, Defects and Stacking Fault Width Analysis. **Journal of Materials Engineering and Performance**, 28(1), 63-78.

17) Talapaneni, T., **Yedla, N**., & Sarkar, S. (2018). Study on desulfurization capacity of high alumina blast furnace slag at 1773 K using slag-metal equilibrium technique. **Metallurgical Research & Technology**, 115(5).

18) Gupta, P., & **Yedla, N.** (2017). Dislocation and Structural Studies at Metal–Metallic Glass Interface at Low Temperature. **Journal of Materials Engineering and Performance**, Volume 26, Issue 12, pp 5694–5704.

19) **Yedla, N.,** Gupta, P., Ng, T. Y., & Geethalakshmi, K. R. (2017). Effect of loading direction and defects on the strength and fracture behavior of biphenylene based graphene monolayer. **Materials Chemistry and Physics**, 202, 127-135.

20) Meraj, M., Dutta, K., Bhardwaj, R., **Yedla, N**., Karthik, V., & Pal, S. (2017). Influence of Asymmetric Cyclic Loading on Structural Evolution and Deformation Behavior of Cu-5 at.% Zr Alloy: An Atomistic Simulation-Based Study. **Journal of Materials Engineering and Performance**, 26(11), 5197-5205.

21) Krishan, J., Gupta, P., Vaduganathan, K., & **Yedla, N**. (2017). Superplastic Pd50Pt50 monocrystalline bimetallic alloy nanowire: a molecular dynamics simulation study. **Metallurgical Research & Technology,** 114(3), 302.

22) **Yedla, N**., & Ghosh, S. (2017). Nature of atomic trajectories and convective flow during plastic deformation of amorphous Cu 50 Zr 50 alloy at room temperature-classical molecular dynamics studies. **Intermetallics**, 80, 40-47.

23) Talapaneni, T., **Yedla, N**., Pal, S., & Sarkar, S. (2017). Experimental and Theoretical Studies on the Viscosity–Structure Correlation for High Alumina-Silicate Melts. **Metallurgical and Materials Transactions B**, 48(3), 1450-1462.

24) Ashwani Kumar, Pradeep Gupta and **Natraj Yedla** (2016) Nanoindentation studies of $Zr_{50}Cu_{50}$ metallic glass thin film nanocomposites via molecular dynamics simulations,

Metallurgical Research & Technology, Vol. 113, p. 602.

25) Pradeep Gupta, Snehanshu Pal, **Natraj Yedla** (2016) Molecular dynamics based cohesive zone modeling of Al (metal)–$Cu_{50}Zr_{50}$ (metallic glass) interfacial mechanical behavior and investigation of dissipative mechanisms, **Materials and Design**, Vol. 105, pp.41-50.

26) Talapaneni, T., **Yedla, N**., Sarkar, S., & Pal, S. (2016). Effect of Basicity, Al2O3 and MgO content on the softening and melting properties of the CaO-MgO-SiO2-Al2O3 high alumina quaternary slag system. **Metallurgical Research & Technology,** 113(5), 501.

27) Patra, A., Meraj, M., Pal, S., **Yedla, N**., & Karak, S. K. (2016). Experimental and atomistic simulation based study of W based alloys synthesized by mechanical alloying. **International Journal of Refractory Metals and Hard Materials**, Vol. 58, pp. 57-67.

28) Meraj, M., **Yedla, N**., & Pal, S. Role of W on the dislocation evolution in Ni-W alloy during tension followed by compression loading. **Met. Mater. Int**., Vol. 22, No. 3 (2016), pp. 373-382.

29) Meraj, M., **Yedla, N**., & Pal, S. (2016). The effect of porosity and void on creep behavior of ultra-fine grained nano crystalline nickel. **Materials Letters**, Vol. 169, pp. 265-268.

30) **Natraj Yedla**, Md. Meraj, Pradeep Gupta, Venumbakkam Sarat, Amar Jyoti Kabi and Snehanshu Pal, The effect of nano-void on deformation behaviour of Al-Cu intermetallic thin film compounds, **Metallurgical Research and Technology**, 2015, Vol. 112, p.505.

31) **N. Yedla**, S. Pal, A. Kumar, Mechanical behaviour of Cu-Zr-Al glassy nano-wires, **Journal of Computational and Theoretical Nanoscience,** 2015, Vol. 12, No 10, p. 2332.

32) Snehanshu Pal, Divya, Zeba Kamal, **Natraj Yedla**, Krishna Dutta, Racheting behaviour of nano-scale copper by classical molecular dynamics simulations, **Journal of Computational and Theoretical Nanoscience**, 2015, Vol. 12, No 9, p. 2264.

33) Srinivasu G., **Natraj Y**., Bhattacharjee, A. Nandy, T.K., NageswaraRao, G.V.S, Tensile and fracture toughness of high strength β-Titanium alloy, Ti–10V–2Fe–3Al, as a function of rolling and solution treatment temperatures, **Materials and Design**, 2013, Vol. 47, p. 323.

34) **Yedla, N**., Srinivas, M., Sudipto, G., Bhaskar, M, Effect of nano-crystallization on the plasticity in Cu-Zr amorphous binary alloys, **Intermetallics**, 2010, Vo. 18, p. 2419.

Publications (Conferences)

1. Kumar, A., Katakareddi, G., & Yedla, N. (2023). High temperature tensile behavior and microstructural evolution in nano-single crystal zirconium: A molecular dynamics simulation study. Materials Today: Proceedings. https://doi.org/10.1016/j.matpr.2023.06.198

2. Katakam, K. C., Gorja, S. R., & Yedla, N. (2023). Experiment and atomistic simulation of

uniaxial compression of Ni–W single-crystal alloy. Materials Today: Proceedings. https://doi.org/10.1016/j.matpr.2023.04.508

3. Katakareddi, G., & **Yedla, N**. (2022). Creep Behavior of Core (Metal)–Shell (Metallic Glass) Structure: a Molecular Dynamics Simulation Study. Transactions of the Indian National Academy of Engineering, 7(2), 405-410.

4. Katakam, K. C., Gorja, S. R., & **Yedla, N**. (2021). Influence of Crystallographic Orientation on the Mechanical Properties and Deformation Behavior of Ni Nanowire Using Large Scale Molecular Dynamics. In Processing and Characterization of Materials (pp. 75-84). Springer, Singapore.

5. Dora, J. K., Saraswat, C., Gour, A., Ghosh, S., **Yedla, N**., & Kundu, T. K. (2021). The role of density reduction in lithiated amorphous silicon: Molecular dynamics and ab-initio studies. Materials Today: Proceedings, 44, 3075-3078.

6. Dora, J. K., Saraswat, C., Gour, A., Ghosh, S., **Yedla, N**., & Kundu, T. K. (2021). The role of density reduction in lithiated amorphous silicon: Molecular dynamics and ab-initio studies. Materials Today: Proceedings.

7. Singh, C., Katakam, K. C., Katakareddi, G., & **Yedla, N**. (2021). Creep behavior of polycrystalline Al (metal)-Cu50Zr50 (metallic glass) cold welds. Materials Today: Proceedings, 41, 316-323.

8. Katakam, K. C., & **Yedla, N**. (2021). Influence of orientation and temperature on the mechanical properties and deformation behavior of nickel nanowire under bending: A large scale molecular dynamics simulation. Materials Today: Proceedings, 39, 1727-1732.

9. Dora, J. K., Ghosh, S., & **Yedla, N**. (2021). Silicon/Acetylene Black–Carbon Composite as an Anode for Lithium-Ion Battery. In Recent Research Trends in Energy Storage Devices (pp. 73-80). Springer, Singapore.

10. Gupta, P., & **Yedla, N**. (2020). Temperature and Loading Rate Effect on the Load-Displacement Response of Metal-Metallic Glass (Al-Cu50Zr50) Layered Structure during Nano-Indentation. In Materials Science Forum (Vol. 978, pp. 330-336). Trans Tech Publications Ltd.

11. Katakam, K. C., & **Yedla, N**. (2020). Deformation Behaviour of Single Linear Surface Defect Nickel Nanowire at Different Temperatures Studied by Molecular Dynamics Simulations. In Materials Science Forum (Vol. 978, pp. 428-435). Trans Tech Publications Ltd.

12. Katakam, K. C., & **Yedla, N**. (2019). Influence Of Single Linear Surface Defect Orientation To Loading Direction In Nickel Nanowire Using Molecular Dynamics In Large Scale. Materials Today: Proceedings, 18, 5472-5480.

13. Gupta, P., & **Yedla, N**. (2018, July). Deformation Behavior and Fracture of Al-CuZr Nano-Laminates: A Molecular Dynamics Simulation Study. In Fracture, Fatigue and Wear (pp. 99-106). Springer, Singapore.

14. Gupta, P., & **Yedla, N**. (2017). Strain Rate and Temperature Effects on the Strength and

Dissipative Mechanisms in Al-Cu 50 Zr 50 Interface Model: Molecular Dynamics Simulation Study. Procedia Engineering, 184, 631-636.

15. Gupta, P., & **Yedla, N**. (2016, February). High Temperature Mechanical Behavior of Aluminum-Cu50Zr50Metallic Glass Interface. In IOP Conference Series: Materials Science and Engineering (Vol. 115, No. 1, p. 012024). IOP Publishing.

16. **N. Yedla**, R. Nalla, S. Pal, P. Gupta and M. Meraj, Molecular Dynamics Studies on the Prediction of Interface Strength of Cu (metal)-CuZr (metallic glass) Metal Matrix Composites, ICMAT 2015, Singapore.

17. Ashwani Kumar and **Natraj Yedla**, Mechanical and structure studies of Zr50Cu50 glass matrix composites during nano-indentation-a molecular dynamics study (2015): IOP Conf. Ser.: Mater. Sci. Eng. 75 012020 doi:10.1088/1757-899X/75/1/012020.

18. Trinath Talapaneni, S Sarkar, **N Yedla** and P L N Reddy (2015), Recovery of Cu and Zn from Complex Sulphide Ore*IOP Conf. Ser.: Mater. Sci. Eng.* 75 012028 doi:10.1088/1757-899X/75/1/012028

19. Subodh Rana, **Natraj Yedla** "Deformation Behavior of Tungsten Nanowire- A Molecular Dynamics Simulation Study " NMD ATM 2013-IT BHU Varanasi.

20. Vidhukesh Vaidehi, **Natraj Yedla** "MD Simulation studies on structure and deformation behavior of FeCoNi metallic glasses" NMD ATM 2013 IT-BHU Varanasi.

21. **NatrajYedla** and SudiptoGhosh, Role of free volume on the plasticity in Cu-Zr amorphous binary alloy, NMD-ATM 2012, Jamshedpur.

22. **Yedla, N.,** and Sudipto Ghosh (2011), Molecular Dynamics Simulation of Plastic Deformation of Metallic Glass at Strain Rates Varying Between 10^{-3} s^{-1} to 10^{1} s^{-1},Advances in Heterogeneous Material Mechanics, 3rd International Conference on Heterogeneous Material Mechanics (ICHMM-2011), Shanghai, China.

23. Ghosh, S.,**Yedla, N**.,Bhaskar, M., Mechanism of plastic deformation and strengthening in Cu-Zr glass: Experimental and MD simulation studies, NMD-2011 Conference held at Hyderabad, India during Nov. 14-17, 2011

Book Chapters

- **Yedla, N**., Salman, S. A., & Karthik, V. (2022). Molecular Dynamics Simulations for Nanoscale Insight into the Phase Transformation and Deformation Behavior of Shape-Memory Materials. **Shape Memory Composites Based on Polymers and Metals for 4D Printing**, 67-80.

Courses Developed

Theory
Computational Modeling of Materials

Laboratory
Computational Modeling of Metallurgical Processes
Molecular Modeling of Materials Deformation Behavior

Research Students

Ph.D.

Guided

1. **Mr. Pradeep Gupta**
   Title: Aluminum-Cu50Zr50 metallic glass interface: Deformation behavior, deformation mechanisms, structure, and fracture studies
2. **Mr. Krishna Chaitanya Katakam**
   Title: Role of Defects on the Deformation Behavior and Mechanisms in Large-Scale Nickel Nanowire Subjected to Different Loading Methods: A Molecular Dynamics Simulation Study

Ongoing

1. **Mr. Ganesh Katakareddi**

M.Tech (Research)

Guided

1. Mr. Ashwani Kumar
   Title: Molecular Dynamics Simulation of Nano-indentation Studies on Zr-based Metallic Glass Matrix Composites.

Personal Details

Date of Birth	20th February, 1980
Residence	FR-39, NIT Campus
Nationality	Indian
Contact No.	Phone: 91-6612462569 (O); 3569 (R)