Dr. Snehanshu Pal

Associate Professor,
Department of Metallurgy and Materials Engineering,
Indian Institute of Engineering Science and Technology, Government of India, Shibpur,
Howrah-711103, West Bengal, India
Website : http://www.snehanshuresearchlab.org/index.html
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Google Scholar Profile: https://scholar.google.co.in/citations?user=1asrimkAAAAJ&hl=en

Profile Summary

Research Areas:	Computational Materials Engineering, Metallurgical Process Modeling and Materials Informatics
Research Profile Keywords:	Atomistic Simulations, Density Functional Theory based simulation Of Energy Materials, Materials Informatics, Steel Making Process, Molecular Dynamics Simulation, Deformation of Metals, Density Functional Theory, Grain Boundary Engineering.
Books Published as author:	Two (2)
Book Published as editor:	One (1)
SCI journal Article Published:	One hundred eight (108)
Doctoral Students Supervised:	Nine (9)
Master Students (M. Tech) Supervised:	Seventeen (17)
Sponsor Research Projects:	Five (5)
Consultancy Research Project:	One (2)
Research/Teaching Experience:	More than Ten years
Industrial Experience (Steel Industry):	More than Three Years

Education

2009-2013 | Ph.D. Metallurgical and Materials Engineering,
Indian Institute of Technology, Kharagpur, India
Research Topic: Atomistic Simulations of Methane Hydrates and Inhibitor Design

1998-2002 | B.E. Metallurgical and Materials Engineering, First Division,
Bengal Engineering college (Deemed University), Shibpore, Howrah, India (currently known as **Indian Institute of Engineering Science and Technology,** Shibpur Howrah, India).

Research /Academic Experience

Sept.2023- Present	Associate Professor, Department of Metallurgy and Materials Engineering, **Indian Institute of Engineering Science and Technology**, Shibpur-711103,India **Research Area:** Computational Materials Engineering, Material Informatics, Process Modeling
Mar.2023- Sept.2023	Assistant Professor, Department of Metallurgical and Materials Engineering, **National Institute Of Technology**, Rourkela-769008,India **Research Area:** Computational Materials Engineering, Material Informatics, Process Modeling
Feb.2014- Mar.2023	Assistant Professor, Department of Metallurgical and Materials Engineering, **National Institute Of Technology**, Rourkela-769008,India **Research Area:** Computational Materials Engineering, Material Informatics, Process Modeling
Sept.2013- Feb.2014	Post-Doctoral Fellow, **Materials Science and Engineering, the Pennsylvania State University,** United States of America(USA) **Research Area:** Computer modeling of heat transfer, material flow in welding process

Industrial Experience

Mar 2006 - July 2009	Organization: **Steel Authority of India Limited, Government of India, India** Department: **Steel Melting Shop of Rourkela Steel Plant, Rourkela, Odisha, India** Designation: **Junior Manager (Operation) – Shift in-charge**

Research Investigator of Sponsored Projects

Principal Investigator

1.**Investigation of solidification process and prediction of microstructure during secondary cooling in continuous casting of plain carbon steel to estimate the porosity fraction and carbon segregated by multi scale simulation (cellular automata and phase field modeling techniques).**
Funding Agency: Department of Science and Technology (DST), Government of India, State Committee on Science and Technology, Belarus.
Total Project Value: INR 8.83 lakhs
Present Status: Completed

2.**The effect of shock wave, moisture and sea water on debonding of multilayer in FRP composite systems -Experimental and multi-scale modeling based investigation**
Funding Agency: Naval Research Board (NRB), DRDO, Government of India
Total Project Value: INR 19.932 lakhs
Present Status: Completed

Research Investigator of Sponsored Project

Co-Principal Investigator

3.**Digitization of steel microstructure images, modelling of plain carbon steel microstructure evolution during heat treatment using cellular automata and phase field modeling methods, and development of a software tool for providing guidance in designing heat treatment process using machine learning based classification techniques**
Funding Agency: Department of Science and Technology, Government of India
Total Project Value: INR 18.546 lakhs
Present Status: Completed

4.**Characterization and numerical simulation of brazed joint - ceramic ring of HVB (High Voltage Bushing)**
Funding Agency: Board of Research in Fusion Science and Technology (BRFST), BRNS, Government of India
Total Project Value: INR 25.64 lakhs
Present Status: Completed

5.**Failure analysis and Cost estimation for AC submerged arc furnace.**
Funding Agency:SARAF Agencies pvt. ltd.
Total Project Value: INR 3.00 lakhs
Present Status: Completed

Research Investigator of Consultancy Project

Principal Investigator	1. **Optimizing minor constituents in blast furnace slag to operate 19-22 percentage slag Alumina** **Funding Agency:** Tata Steel Ltd. **Total Project Value:** INR 19.90 lakhs **Present Status:** Completed
Principal Investigator	2. **Investigation on Hydrogen Diffusion in High Entropy Alloy** **Funding Agency:** CSIR- Indian Institute of Petroleum **Total Project Value:** INR 3.00 lakhs **Present Status:** Completed

Achievements

Ranked 30th (all India rank) in Graduate Aptitude Test in Engineering (GATE) 2009

Courses Taught as Course Teacher

Subject No.	Subject Name	L-T-P
MM611	Process Modelling for Steel Industry	3-0-0
MM6311	Metallurgical Thermodynamics and Kinetics	3-0-0
MM2302	Transport Phenomenon	3-0-0
MM472	Thermodynamic Modeling of Metallic systems	0-0-3
MM305	Steel Making	3-0-0
MM426	Secondary Steel Making	3-0-0
MM274	AtomisticModellingof Materials Laboratory	0-0-3
MM476	Computational Modeling of Process Metallurgy Laboratory	0-0-3
MM494	Seminar and Technical Writing – II	0-0-0

Supervised Ph.D. Thesis Works as A single/sole supervisor (Total No. 2)

Degree and year	Title of Thesis	Name of the Student
Ph.D. (2019) Degree awarded	Molecular Dynamics Simulation Based Study for Creep Deformation Behaviour of Nanocrystalline Nickel and Nickel-Zirconium Alloys	Dr. Md. Meraj (**Obtained Institute Gold Medal for the best Ph.D.Thesis of 2019-20 in National Institute of Technology Rourkela , India**)
Ph.D. (2021) Degree awarded	Molecular Dynamics Simulation Of Deformation Behaviour During Nanoscale Rolling	Dr. K. Vijay Reddy
Ph.D. (2023) Degree awarded	Molecular dynamics simulation of deformation behavior of Al90Sm10 metallic glass and Al-Al90Sm10 crystalline-amorphous nanolaminate	Dr. S. Mishra

Supervised Ph.D. Thesis Works as A joint supervisor (Total No. 6)

Degree and year	Title of Thesis	Name of the Student
Ph.D. (2018) Degree awarded	Fabrication of Nano-Y2O3 Dispersed Tungsten Alloys by Mechanical Alloying Followed by Conventional and Spark Plasma Sintering	Dr. A. Patra
Ph.D. (2020) Degree awarded	Laser weld-brazing of aluminum alloy (AA6082/AA5083) and galvanized interstitial free steel with an emphasis on fatigue and corrosion study	Dr. N. Chary
Ph.D. (2021) Degree awarded	Investigation of Deformation Behavior of High Entropy Alloy Coated FCC Metallic Systems under Nanoindentation using Molecular Dynamics Simulation	Dr. D. Mishra
Ph.D. (2022) Degree awarded	Refinement and Processing of Steel Microstructure Images Facilitating Automated Heat Treatment Process Prediction	Dr. A Panda
Ph.D. (2023) Degree awarded	Molecular dynamics simulation of deformation Behavior of nanocrystalline Al and CNT reinforced nanocrystalline Al nanocomposites	Dr. P N Babu
Ph.D. (2023) Degree awarded	The effect of shock wave, moisture and sea water on de-bonding of multilayer in FRP composite systems experimental and multi-scale modeling based investigation	Dr. S. Gupta

Supervised M. Tech Thesis Works (Total No. 13)

Degree and year of degree awarded	Title of Thesis	Name of the Students
M.Tech (2023)	Optimizing minor constituents in blast slag to operate 19-22 percentage slag Alumina using material informatics approach	Mr. Devi Dutta Biswajeet
M.Tech (2022)	Evaluation of structural properties and thermoelectric properties of quaternary oxides.	Mr. Ginnarapu Shivakrishna
M.Tech (2022)	Investigation of molecular interaction of protein with hydroxyapatite surface using atomistic scale computational modelling technique.	Mr. Saurav Singh
M.Tech (2022)	Molecular Dynamic Simulation of Mechanical Behaviour of Magnesium during Nano-indentation and Ballistic Penetration	Mr. Pragyan Goswami
M.Tech (2020)	Molecular Dynamic Simulation of Nano Scale Friction Stir Welding	Mr. Roshan Kumar Jha
M.Tech (2019)	Modelling of trajectory of steel droplet and determination of residence time in slag during steel refining process using CFD	Mr. Prabhash Kumar
M.Tech (2018)	Modeling of solidification process and estimation of carbon segregation occurred during secondary cooling stage of continuous casting process of plain carbon steel	Mr. Gaddam Vishal
M.Tech (2018)	Optimization of Ferrochrome Addition Using Multi-Objective Evolutionary and Genetic Algorithms for Stainless Steel Making via AOD Converter	Mr.Kishore Kumar Behera
M.Tech (2017)	Mechanical performance evaluation of woven and unidirectional GFRP composite through numerical simulation	Mr. Yogesh Shamsundar Mhetre
M.Tech (2017)	Finite Element Analysis for adhesive bonding strength of steel and FRP composite joint	Mr. Bansal Darji VinayKumar
M.Tech (2016)	The Influence of Chromium Amount, Casting Speed and Superheat on The Columnar to Equiaxed Transition and Metallurgical Length for Continuously Cast Ferritic Stainless Steels	Mr. Ritesh Padhi
M.Tech (2016)	Dynamic process modeling of stainless steel making through AOD converter	Mr. Jagdish Nayak
M.Tech (2016)	Prediction of microstructure for heat treatment process in dual phase steels using Cellular Automata	Mr. Vijay Reddy
M.Tech (2016)	Numerical Study of Post Welds Residual Stress and Creep Behavior of Inconel 718 and 316 Stainless Steel Joints	Mr. Bhardwaj Ravindra Giriraj
M.Tech (2015)	Computational Fluid Dynamic (CFD) simulation for continuous casting process of steels	Mr. RahulKumar
M.Tech (2015)	Mathematical Modelling of Basic Oxygen Steel Making Process	Miss Vinita Kumari

Supervised B. Tech Thesis Works (Total No. 21)

Degree and year	Title of Thesis	Name of the Students
B.Tech (2023)	Financial Spectrum of Boeing 737 and its Dependence on Component-wise Material Selection.	Aayush Dinesh Kandpal
B.Tech (2023)	A Molecular Dynamics Study of Shock Induced Viscosity of Fe-Cr Alloys using Green Kubo relation and its Dependence on Temperature.	Shantanu Khawas
B.Tech (2023)	Machine learning based phase prediction model for multi-principal element alloys and web based application development.	Neeraj Kumar
B.Tech (2023)	Interfacial diffusion behaviour bimetallic system.	Sudeeksha Vandrangi
B.Tech (2022)	Dynamic assessment of grain boundary, solute and dislocation interaction in FCC metal	Tapashree Pradhan
B.Tech (2022)	Effect of Grain Boundary and Interficial Energy Anisotropy on Ternary Phase Separation	Abhinav Roy
B.Tech (2021)	Simplementation of machine Learning for coordinating among process variable, composition and turn down Temperature for Basic Oxygen Steel making process.	Suraj Hansdah
B.Tech (2021)	Study of Dislocation Precipitate Interaction in Ni-Al System Through Molecular Dynamic Simulation.	Nichenametla Jai Sai
B.Tech (2021)	Ab-initio prediction and analysis of novel d0 Heusler alloys.	Adesh Rohan Mishra
B.Tech (2021)	Molecular Dynamics simulation-based study on the shock response of Ni bicrystals	Tanmay Konnur
B.Tech (2020)	Study of Fluid Flow Behaviour in Secondary Steel making using computational fluid dynamics	Dibya Ranjan Sahoo
B.Tech (2019)	Study of creep behavior of Ni62Nb38 metallic glass	B Anjali
B.Tech (2019)	Creep-ratcheting interaction study of nanocrystalline nickel using atomistic simulation	Sushrita Dash
B.Tech (2019)	Evolution of dislocation density in the Ni(metal) -NiTi(metallic glass) interface with the variation in interfacial area and size of the sample	Priyansha Nikita
B.Tech (2018)	Influence of Dislocation density and grain size on precipitation kinetics in P92 grade steel	Karanam Gururaj
B.Tech (2018)	Influence of specimen size and strain rate on tensile deformation and fracture behavior of single-layer Silicene	B.S.K. Gargeya

Supervised B. Tech Thesis Works (Total No. 21) continued..

Degree and year	Title of Thesis	Name of the Students
B.Tech (2017)	Attempt to identify strategy for micro structure modelling of low carbon steel	Mr.Ankit Surana
B.Tech (2017)	The influence of void and porosity on deformation behaviour of nanocrystalline Ni under tensile followed by compressive loading	Mr.Kumar Krishanjeet
B.Tech (2017)	Microstructure prediction during Inter Critical Heating and Subsequent Cooling of Low Carbon Steel	Mr.Ayush Poddar
B.Tech (2016)	Process For Extraction of Titanium Oxide From Ilmenite Ore by Application of Coke	Mr.Anurag Mishra
B.Tech (2015)	Density Functional Theory Based Investigation of 1- Butyl-3-Methylidazolium as a Potential Methane Hydrate Inhibitor	Mr.Satyam Choudhury

Referee or Reviewer for the Journals

1. Computational Material Science
2. Steel Research International
3. Acta Materilia
4. Journal of Materials Engineering and Performance
5. Intermetallics
6. Engineering Computation
7. Journal of Materials Science and Technology
8. Materials Chemistry and Physics
9. International Journal of Mechanical Sciences
10. Journal of Alloys and Compounds
11. Journal of Material Research and Technology
12. Nature Communications
13. Modelling and Simulation in Materials Science and Engineering
14. Machine Learning: Science and Technology
15. Journal of Nanostructure in Chemistry
16. Indian Institute of Metals Transactions
17. Journal of Molecular Modeling
18. Materials Letters
19. Journal of Physics: Condensed Matter
20. Journal of Applied Physics
21. Sadhana
22. Emergent Materials
23. International Journal of Energy Research
24. Journal of Non-crystalline Solids
25. Mechanics of Materials
26. Advances and Applications in Bioinformatics
27. Computational Condensed Matter
28. Engineering Failure Analysis

29. Journal of Materials Research
30. Signal Processing: Image Communication
31. Journal of Institute of Engineers(India): Series C
32. Materials & Design
33. Applied Physics A
34. The European Physical Journal B
35. Chemical Engineering Science
36. Journal of Computational Design and Engineering
37. Journal of Materials Science
38. Physica Scripta

Invited Talk/Lecture

1. Themed Tech Talk on "Scope of Interdisciplinary Research" by **Snehanshu Pal (Invited Speaker)** on December 17th 2018 organised by Intelligent Systems Research Group, School of Computer Science, UPES, Dehradun (India)

2. Lecture on "Advancement in Steel Making: Industrial Prospective" by **Snehanshu Pal (Invited Speaker)** on October 1st 2018 in the workshop titled "Advancement in Iron and Steel Making: Industrial Prospective" organised by Department of Metallurgical and Materials Engineering, OPJU, Raigarh (India)

3. Talk on "Quality Assessment through Information and Modeling for Composite Materials" by **Snehanshu Pal (Invited Speaker)** on Workshop 17th- 18th May 2018 organised by Tata Steel, Jamshedpur (India)

4. "Creep Behaviour Study of Nano-crystalline Stainless Steel and Nano-crystalline Nickel Join Using Molecular Dynamics Simulation" By Md. Meraj and **Snehanshu Pal (Keynote Speaker and Corresponding Author)**, 4th International Conference on Thermo-mechanical Simulation and Processing of Steels (Simpro'2016), February 10th- 12th 2016, RDCIS, SAIL, Ranchi (India)

5. Lecture on "Application of Computational Materials Engineering on Materials Characterization and Property Evaluation" by **Snehanshu Pal (Invited Speaker)** in Technical Education Quality Improvement Programme (TEQIP-II) sponsored Workshop on "Advanced Techniques in Materials Characterization" on 22nd- 23rd January 2016 organized Department of Metallurgical Engineering, NIT Raipur

Book Published as author(Total No. 2)

2. "Molecular Dynamics Simulation of Nanostructured Materials An Understanding of Mechanical Behavior", **Snehanshu Pal**, Bankim Chandra Ray, ISBN: 9780367029821, CRC Press, Boca Raton, USA, **2020**.

1. "Process Modeling for Steel Industry", **Snehanshu Pal**, Anshuman Patra, Prabodh Ranjan Padhee, ISBN : 9789385909399, I.K. International Publishing House Pvt. Ltd, India, **2018**.

Book Published as editor(Total No. 1)

1. "Processing and Characterization of Materials", **Dr.Snehanshu Pal**, Dr. Debdas Roy, Dr. Sudip Kumar Sinha, ISBN: 9789811639364,Springer Nature, Singapore Pte Ltd.,**2021**.

Published Book Chapter

1. Book chapter title "Dynamic Structural Evolution of Nanocrystalline Aluminum During Ratcheting Deformation" by P. Narendra Babu, K. V. Reddy and **Snehanshu Pal** of the Book, titled "Nano Scaled Structural Problems: Static and Dynamic Behaviors", Chapter no. 6 , ISBN: 9780735422865006, AIP Publishing (2021).

2. Book chapter title "Creep Behaviour Study of Nano-crystalline Stainless Steel and Nanocrystalline Nickel Join Using Molecular Dynamics Simulation" by Md. Meraj and **Snehanshu Pal** of the Book, titled "Thermo-Mechanical Simulation and Processing of Steels", Chapter no. 14 , ISBN: 978-93-85919-86-2, Viva Books Private Limited (2016).

3. Book chapter title "CFD Modeling of Fluid Flow Behavior and Bath Surface Deformation in LD Converter" by T. K. Kundu and **Snehanshu Pal** of the Book, titled "CFD Modeling and Simulation in Materials Processing", Chapter no. 38 , ISBN: 978-1-1182-9615-8 , Wiley online library (2012).

SCI Journal Article Publications (Total No. 108)

2023:

108. " Atomistic simulation of rolling contact fatigue behavior of a face-centered cubic material (nickel)", P. Goswami, **S. Pal (Corresponding Author)**, M. Gupta,**Fatigue and Fracture of Engineering Materials and Structures** (2023). DOI: 10.1111/ffe.14196

107. " Investigation on wear-resistance of nanocrystalline Pt-Au by molecular dynamics simulations", T. Pradhan, **S. Pal (Corresponding Author)**, C. Deng,**Tribology International** Vol. 189, pp. 108966 (2023)

106. " A molecular dynamic simulation-based study on nanoscale friction stir welding between copper and aluminium", R. K. Jha, K. V. Reddy, **S. Pal**, **Molecular Simulation**, pp. 1-12 (2023)

105. " Correlation and Prediction of Molten Steel Temperature in Steel Melting Shop Using Reliable Machine Learning (RML) Approach ", M. K. Singh, A. Choudhury, D. Uikey, **S. Pal**,**Transaction of the Indian Institute of Metals** Vol. 76, pp. 3365–3377 (2023)

104. " Unveiling the effect of interface on torsional behavior of crystalline Al-Al90Sm10 metallic glass nanolaminates ", S. Mishra, **S. Pal (Corresponding Author)**, **Philosophical Magazine** Vol. 103, pp. 1-24 (2023)

103. " Optimization of high alumina slag practice in blast furnace ironmaking: an industrial approach. Part 2: Data-driven aspects ", **S. Pal**, M. Sahoo, D.D. Biswajeet, S. Hazra, G.S. Tarachand, D. Bhattacharyya, S. Nag, S. Seetharaman, **Journal of Ironmaking and Steelmaking** Vol. 50, pp. 1-14 (2023)

102. " Optimization of high alumina slag practice in blast furnace ironmaking: an industrial approach (PART 1: fundamental aspects) ", S. Hazra, **S. Pal**, D.D. Biswajeet, M. Sahoo, G.S. Tarachand, D. Bhattacharyya, S. Nag, S. Seetharaman, **Journal of Ironmaking and Steelmaking** Vol. 50, pp. 1-14 (2023)

101. " Molecular dynamics simulation for radiation response of Nb bicrystal having 13, 29, and 85 grain boundary ", M. Manna,**S. Pal (Corresponding Author)**, **Journal of**

Applied Physics Vol. 133, pp. 165902 (2023)

100. " Molecular dynamics study of nano-indentation deformation behavior of Al/Al90Sm10 nanolaminate ", S. Mishra, **S. Pal (Corresponding Author)**, **Journal of Molecular Modeling** Vol. 29, pp. 112 (2023)

99. " An overview of mechanical properties and failure mechanism of FRP laminates with hole/cutout ", S. Gupta,**S. Pal**, B.C. Ray, **Journal of Applied Polymer Science** Vol. 140, pp. 1-20 (2023)

98. " Atomistic insight of torsional behavior of CNT-nanocrystalline Al nanocomposites ", P.N. Babu, B.S.K. Gargeya, B.C. Ray,**S. Pal (Corresponding Author)**, **Diamond and Related Materials** Vol. 134, pp. 109768 (2023)

2022:

97. " Investigation of point defect evolution and Voronoi cluster analysis for magnesium during nanoindentation. ", P. Goswami, **S. Pal**, M. Gupta, **Journal of Magnesium and Alloys** Vol. 11, pp. 1029-1042 (2022)

96. "Dislocation entangled mechanisms in cu-graphene nanocomposite fabricated by high-pressure sintering. ", N. Khobragade, T. Maity, A. widerska- roda, G. Stanislaw, W. ojkowski, P. N. Babu, **S. Pal**, D. Roy, **Materials Characterization** Vol. 195, pp. 112524 (2022)

95. "Molecular dynamics simulation on creep-ratcheting behavior of columnar nanocrystalline aluminum. ", P. N. Babu, **S. Pal (corresponding author)**, **Journal of Molecular Graphics and Modelling** Vol. 118, pp. 108376 (2022)

94. "Improvement in radiation resistance of nanocrystalline Cu using grain boundary engineering: an atomistic simulation study. ", M. Manna, **S. Pal (corresponding author)**, **Journal of Materials Science** Vol. 57, pp. 19832–19845 (2022)

93. "Atomistic assessment of structural evolution for magnesium during hypervelocity nanoprojectile penetration. ", P. Goswami, M. Gupta, **S. Pal (corresponding author)**, **Journal of Molecular Modeling** Vol. 28(11), pp. 1-11 (2022)

92. "An analysis on tensile and flexural loading response for unidirectional CFRP laminate with cutout/hole: Geometrical design effect on the material strength. ", S. Gupta, **S. Pal**, , B. C. Ray, **Journal of Applied Polymer Science** Vol. 139, pp. e53139 (2022)

91. "Tailoring structural inhomogeneities in Al90Sm10 metallic glass nanowire via torsional deformation", S. Mishra, **S. Pal**, **Journal of Non-Crystalline Solids**, Vol. 595, pp.121830 (2022)

90. " Improving thermal stability and Hall-Petch breakdown relationship in nanocrystalline Cu: A molecular dynamics simulation study ", **S. Pal (corresponding author)**, K. Vijay Reddy, C. Deng, **Materials Letters** Vol. 324, pp. 132821 (2022)

89. " Small-scale deformation behaviour of the AlCoCrFeNi2.1 eutectic high entropy alloy ", S. K. Singh, G. Kumar, P. N. Babu,**S. Pal**, S. Vashistha, M. S. Azam S. Dixit, **Philosophical Magazine** Vol. 17, pp. 1708-1724 (2022)

88."Generative Adversarial Networks for Noise Removal in Plain Carbon Steel Microstructure Images", A. Panda,R. Nashar, **S. Pal, IEEE Sensors Letters**, Vol. 6, pp. 1-4(2022)

87."Atomistic Insight into the Texture Weakening and Shear-Shuffle Twinning Mechanism During Cold-Rolling of Magnesium", K. V. Reddy, **S. Pal (corresponding author), JOM** Vol.74, pp.1387–1394 (2022)

86. "Amorphous Intergranular Film Effect on the Texture and Structural Evolution During Cold-Rolling of Nanocrystalline Ni–Zr Alloys", K. V. Reddy, T. J. Rupert, **S. Pal (corresponding author), Metallurgical and Materials Transactions A**, Vol. 53, pp.1025–1034 (2022)

2021:

85. "Stable nanocrystalline structure attainment and strength enhancement of Cu base alloy using bi-modal distributed tungsten dispersoids", D. Roy, **S. Pal**, C. S. Tiwary, A. K. Gupta, P.N. Babu, R. Mitra, **Philosophical Magazine**, (2021)

84. "Ab-initio investigation of structural, mechanical, thermodynamic, electronic, magnetic and thermoelectric properties of half-metallic d0 half-Heusler alloys LiXSi (X=Ca, Sr)", A. R. Mishra, **S. Pal (corresponding author), Journal of Solid State Chemistry**,Vol. 304, pp. 122610-1, (2021)

83. "Impact of crystalline–amorphous interface on shock response of metallic glass Al90Sm10 crystalline Al nanolaminates", S. Mishra, K. V. Reddy, **S. Pal (corresponding author), Applied Physics A**, Vol 127 (2021)

82. "Investigation of structural evolution in the Cu–Zr metallic glass at cryogenic temperatures by using molecular dynamics simulations", A. A. Deshmukh, J. G. Bhatt, P. M. Gade, **S. Pal, Journal of Molecular Modeling**, Vol 27, (2021)

81. "Cold-rolling induced residual stress effect on the shock response of crystalline-metallic glass (Cu–CuZr) nanolaminates by molecular dynamics simulation" K. V. Reddy, **S. Pal (Corresponding Author)**, **Materials Chemistry and Physics**,Vol. 272, 125010 (2021)

80. "Investigation of lanthanide complexation with acetohydroxamic acid in nitrate medium: experimental and DFT studies" A. Pati,A. Bhattacharyya, P.K. Pujari, **S. Pal**, T. K. Kundu **Journal of Chemical Sciences**,Vol. 133,(2021)

79. "Correlation and Optimization of Phosphorus Content in Liquid Steel with Turndown Temperature and FeO Content in Slag for Steel Making by LD Converter by Implementing Multi-Objective Evolutionary and Genetic Algorithms" M, K. Singh, C. Halder, S. Dixit, **S. Pal**, **IIM Transactions**,(2021)

78. "Recreating the shear band evolution in nanoscale metallic glass by mimicking the atomistic rolling deformation: a molecular dynamics study" K. V. Reddy, **S. Pal (Corresponding Author)**, **Journal of Molecular Modeling**,Vol. 27, pp. 220 (2021)

77. "Atomistic simulation of crack propagation in CNT reinforced nanocrystalline aluminum under uniaxial tensile loading" P. N. Babu, S. Dixit, , **S. Pal (Corresponding Author)**, **Philosophical Magazine**,(2021)

76. "First-principles calculations to investigate electronic structure and magnetic, mechanical and thermodynamic properties of d0 half-Heusler LiXN (X= Na, K, Rb) alloys" A. R. Mishra, **S. Pal (Corresponding Author)**, **Solid State Sciences**,Vol. 118, pp. 106633 (2021)

75. "Effect of variation in inclination angle of 5 tilt grain boundary on the shock response of Ni bicrystals" T.Konnur, K. V. Reddy, **S. Pal (Corresponding Author)**, **Applied Physics A**,Vol. 127, pp. 358 (2021)

74. "The spectrum of atomic excess free volume in grain boundaries" **S. Pal**, K. V. Reddy, T. Yu, J. Xiao, C. Deng, **Journal of Materials Science**,Vol. 56, pp. 11511–11528 (2021)

73. "Constant twist rate response of symmetric and asymmetric 5 aluminium tilt grain boundaries: molecular dynamics study of deformation processes" B.S. K. Gargeya, P. N.

Babu, **S. Pal (Corresponding Author)**, **Journal of Materials Science**,Vol. 56, pp. 8544–8562 (2021)

2020:

72. "Bi-objective Optimization of Maraging Steel Produced by Vacuum Induction Melting Using Evolutionary Algorithms, " C. Halder, L. P. Kuppili, S. Dixit, **S. Pal** , S. K. Jha, **Transactions of the Indian Institute of Metals**, (2020)

71. " Atomistic Simulation of Nano-Rolling Process for Nanocrystalline Tungsten" K.V. Reddy, **S. Pal (Corresponding Author)**, **JOM : Journal of The Minerals, Metals, and Materials**, Vol. 72, pp. 3977–3986 (2020)

70. " Molecular dynamics simulation-based study of creep–ratcheting behavior of nanocrystalline aluminum," P.N. Babu, C.S Becquart **S. Pal (Corresponding Author)**,**Applied Nanoscience**, Vol.11, pp. 565–581 (2020)

69. "Influence of rolling temperature on the structural evolution and residual stress generation of nanocrystalline Nickel during nano-rolling process" K.V. Reddy, **S. Pal (Corresponding Author)**, **Computational Materials Science**, Vol. 184, pp. 109935-1 (2020)

68. "Accumulative roll bonding of Cu–Zr nanolaminate: Atomistic-scale investigation of structural evolution and grain orientation scatter dependence on rolling parameters" K.V. Reddy, **S. Pal (Corresponding Author)**, **Journal of Applied Physics**, Vol.127, pp. 154305-1 (2020)

67. " Strength degradation and fractographic analysis of carbon fiber reinforced polymer composite laminates with square / circular hole using scanning electron microscope micrographs" S. Gupta, R. K. Prusty, B. C. Ray **S. Pal**, **Journal of Applied Polymer Science**, Accepted (2020)

66. "Dynamic probing of structural evolution for Co50Ni50 metallic glass during pressurized cooling using atomistic simulation ", A. A. Deshmukh, **S. Pal (Corresponding Author)**, **Journal of Molecular Modeling**, Vol.26,(2020)

65. "A potential insight into the serration behaviour of Sigma3 power n (n less than equal 3) boundaries in Alloy 617" P. Bhuyan, K.V. Reddy, S.K. Pradhan, **S. Pal**, R.Mitra, S. Mandal, **Materials Chemistry and Physics**, Vol.248, pp. 122919-1 (2020)

64. "Zr segregation in Ni–Zr alloy: implication on deformation mechanism during shear loading and bending creep" **S. Pal (Corresponding Author)**, K. Vijay Reddy, Douglas E. Spearot, **Journal of Materials Science**, Vol.55, pp. pages 6172–6186 (2020)

63. "Molecular Dynamics simulation based investigation of possible enhancement in strength and ductility of nanocrystalline aluminum by CNT reinforcement" **S. Pal (Corresponding Author)**, P. Narendra Babu, B.S.K.Gargeya, C. S.Becquart, **Materials Chemistry and Physics**, Vol.243, pp. 122593-1 (2020)

2019:

62. "Structure prediction of multi-principal element alloys using ensemble learning" A. Choudhury, T. Konnur, P.P. Chattopadhyay, **S. Pal (Corresponding Author)**, **Engineering Computations**, Accepted (2019)

61. "Shock velocity-dependent elastic-plastic collapse of pre-existing stacking fault tetrahedron in single crystal Cu" K. Vijay Reddy, **S. Pal (Corresponding Author)**, **Computational Materials Science**, Vol. 172, pp. 109390-1 (2019)

60. "Atomistic study of fracture behavior of metallic glass fiber reinforced metal-matrix nanocomposite during bending creep deformation process" K. Vijay Reddy, **S. Pal (Corresponding Author)**, **International Journal of Materials Research**, Vol. 110, pp. 1142-1149 (2019)

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58. "Intensification of shock damage through heterogeneous phase transition and dislocation loop formation due to presence of pre-existing line defects in single crystal Cu" K. Vijay Reddy, C. Deng, **S. Pal (Corresponding Author)**, **Journal of Applied Physics**, Vol 126, pp. 174302-1 (2019)

57. "Atomistic investigation of the deformation mechanisms in nanocrystalline Cu with amorphous intergranular films" A. H. Neelav, S. Pal, C. Deng, **Journal of Applied Physics**, Vol 126, pp. 125101-1 (2019)

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53. "Molecular Dynamics Simulation Study of Uniaxial Ratcheting Behaviors for Ultrafine-Grained Nanocrystalline Nickel"**S. Pal (Corresponding Author)**, K. Gururaj, Md. Meraj, and R. G. Bharadwaj, **Journal of Materials Engineering and Performance**, Vol. 28, pp. 4918

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41. "Optimisation between tundish temperature and slab exit temperature to eliminate "strand stuck-up" phenomenon in continuous casting process of steel by implementation of multi-objective evolutionary and genetic algorithm". **S Pal (Corresponding Author)**, Kishore Kumar Behera, Prabodh Ranjan Padhee, Smarajit Sarkar, Chandan Halder, **Steel Research International** , (Accepted, 2018)

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21. "Healing Mechanism of Nanocrack in Nanocrystalline Metals during Creep Process", M. Meraj, **S Pal (Corresponding Author)**, **Applied Physics A**, Vol. 123(2), pp. 138 (2017)

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

19."Mechanistic study of bending creep behaviour of bicrystal nanobeam" K. Vijay Reddy, M Meraj, **S Pal (Corresponding Author)**, **Computational Materials Science**, 136, pp. 36—43 (2017)

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17. "AA6082 to DX56-Steel Laser Brazing: Process Parameter–Intermetallic Formation Correlation" D. Narsimhachary, S. Pal, S. M. Shariff, G. Padmanabham, A. Basu, **Journal of Materials Engineering and Performance**, Vol. 26, pp. 4274-4281 (2017)

16. ""Processing and refinement of steel microstructure images for assisting in computerized heat treatment of plain carbon steel." S Gupta, A Panda, R Naskar, D Mishra, **S. Pal**, **Journal of Electronic Imaging**, Vol. 26, pp. 063010 (2017)

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14. "The effect of porosity and void on creep behaviour of ultra-fine grained nano crystalline nickel", Meraj, N. Yedla and **S Pal (Corresponding Author)**, **Materials Letters** Vol. 169, pp. 265-268 (2016)

13. "Molecular Dynamics based Cohesive Zone Modelling of Al(metal)-Cu50Zr50 (metallic glass) interfacial mechanical behaviour and investigation of dissipative mechanism", Pradeep Gupta, **S Pal** and N. Yedla, **Materials and Design**, Vol. 105, pp. 41- 50 (2016)

12. "Optimization of phosphorous in steel produced by basic oxygen steel making process using multi-objective evolutionary and genetic algorithms", **S Pal (Corresponding Author)**, C. Halder, **Steel Research International**, Vol. 88(3), pp. 1600193 (2016)

11. "Role of W on the Deformation behaviour of Ni-W Alloy under Tensile Followed by Compressive Loading" M Meraj, N. Yedla, **S Pal (Corresponding Author)**, **Metals and Materials International**, Vol.22 (3),pp. 373-382(2016)

10. "The Effect of Temperature on Creep Behaviour of Porous (1 at.percent) Nano Crystalline Nickel". M. Meraj and **S Pal (Corresponding Author)**, **Transactions of the Indian Institute of Metals**, Vol. 69, pp. 277-282 (2016)

9. "Electrophoretic deposition of Cu-SiO2 coatings by DC and pulsed DC for enhanced surface mechanical properties", H.S. Maharana, S. Lakra, **S. Pal**, and A. Basu, **Journal of Materials Engineering and Performance**, Vol. 25, No. 1, pp. 327- 337(2016)

8. "Surface-Mechanical Properties of Electrodeposited Cu-Al2O3 Composite Coating and Effects of Processing Parameters". HS Maharana, A Ashok, **S Pal**, A Basu, **Metallurgical and Materials Transactions A**, 47A, pp. 388—399 (2016)

7. "Effect of basicity, Al2O3 and MgO content on the characteristic temperatures of the CaO-MgO-SiO2-Al2O3 high alumina quaternary slag system". T. Trinath, N. Yedla, S. Sarkar, **S Pal**, **Metallurgical Research Technology**, Vol. 113(5), pp. 501 (2016)

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

2015:

5."Asymmetry in steel welds with dissimilar amounts of sulfur", H. L. Wei, **S. Pal**, V. Manvatkar, T. J. Lienert, and T. DebRoy. **Scripta Materialia**, Vol. 108, pp. 88- 91 (2015)

4. "The effect of nano-void on deformation behaviour of Al-Cu intermetallic thin film compounds", N. Yedla, M. Meraj, P. Gupta, V. Sarat, A. J. Kabi and **S Pal (Corresponding Author)**, **Metallurgical Research Technology**, Vol. 112, pp. 505 (2015)

2014:

3. "Design of methane hydrate inhibitor molecule using Density Functional Theory." **S Pal (Corresponding Author)** and T. K. Kundu, **Journal of Cluster Science**, Vol. 2, pp. 551-563(2015)

2013:

2. "Pentagonal dodecahedron methane hydrate cage and methanol system - an Ab initio study" by **S Pal (Corresponding Author)**, T. K. Kundu, **Journal of Chemical Science**, Vol. 125, pp. 379–385 (2013)

1. "DFT based inhibitor and promoter selection criteria for pentagonal dodecahedron methane hydrate cage" **S Pal (Corresponding Author)**, T. K. Kundu, **Journal of Chemical Science**, Vol. 125, pp. 1259 -1266 (2013)

Conference Presentations

1. "An anomaly in creep property dependence on grain size for ultrafine grain nanocrystalline Nickel at higher creep temperature", Md. Meraj (Presenter), Snehanshu Pal, 2nd International Conference on Science and Engineering of Materials (ICSEM-2018), January 6-8, 2018, Sharda University (India).

2. "Effect of temperature on creep behavior of nanocrystalline Ni having multimodal grain distribution with pre- existing crack", Md. Meraj (Presenter), Snehanshu Pal, The 9th International Conference on Materials for Advanced Technologies (ICMAT-2017), June 18-23, 2017, Suntec Exhibition Center (Singapore).

3. "Analysis of deformation behaviour of Al-Ni-Co thin film during nanoindentation: A Molecular Dynamics study", K. Vijay Reddy (Presenter), Snehanshu Pal, 17th International Conference on Thin Films (ICTF-2017), November 13-17, 2017, CSIR-National Physical Laboratory, New Delhi (India).

4. "Molecular Dynamics simulation based study of the tensile loading behaviour of Silicene", B.S.K. Gargeya (Presenter), Snehanshu Pal, International Conference on Nanotechnology: Ideas, Innovations Initiatives (ICN:3I-2017), December 6-8, 2017, Indian Institute of Technology Roorkee (India).

5. "An atomistic simulation based investigation on the influence of Zr addition on deformation behavior of nanocrystalline Ni", Md. Meraj (Presenter), B.S.K. Gargeya, K. Vijay

Reddy, Snehanshu Pal, 10th International Conference on Precision, Meso, Micro and Nano Engineering (COPEN 10), December 7-9, 2017, Indian Institute of Technology Madras (India).

6. "The Effect of Temperature on Creep Behaviour of Porous (1 at.Crystalline Nickel", M. Meraj (presenter) and S. Pal (Corresponding Author), 7th International Conference on Creep, Fatigue and Creep - Fatigue Interaction (CF-7)-2016, January 19-22, 2016, Indira Gandhi Centre for Atomic Research Kalpakkam (India).

7. "Deformation of Ni20W20Cu20Fe20Mo20 high entropy alloy for tensile followed by compressive and compressive followed by tensile loading: A molecular dynamics simulation based study", M. Meraj (presenter) and S. Pal (Corresponding Author) , 5th National Conference on Processing Characterization of materials 12-13th December, 2015 National Institute of Technology, Rourkela (India).

8. "Multiphase Computational Fluid Dynamics (CFD) modeling study of slopping behavior during basic oxygen steel making (BOS) process", S. Pal (presenter and Corresponding Author) , V. Kumari, R. Kumar and N. Yedla, KomPlasTech 2015- XXII International Conference Computer Methods in Materials Technology - January 11 -14, 2015, Krynica-Zdrój (Poland)

9. "Molecular Dynamics Studies on the Prediction of Interface Strength of Cu (metal)-CuZr (metallic glass) Metal Matrix Composites", N. Yedla (presenter), R. Nalla, S. Pal, P. Gupta and M. Meraj, 8th International Conference on Materials for Advanced Technologies of the Materials Research Society of Singapore IUMRS – International Conference in Asia (ICMAT2015 IUMRS-ICA2015), 28 June - 3 July 2015, Suntec (Singapore).

10. "Theoretical study of methanol as inhibitor and cyclopentane as stabilizer of dodecahedron methane hydrate cage." S. Pal (presenter and Corresponding Author), and T. K. Kundu. In IOP Conference Series: Materials Science and Engineering, vol. 73, no. 1, p. 012081. IOP Publishing, 2015.

11. "Density Functional Theory Study of Methane Encapsulation in Different Clathrate Hydrate Cage Structure" by S. Pal (presenter and Corresponding Author) ,and T. K. Kundu International Conference on Advances in Materials and Materials Processing (ICAMMP) 2011 Oral Presentation Volume (2011)

12. "Comparative Stability Analysis of Different Methane Hydrates Structures Using Density Functional Theory" by S. Pal and T. K. Kundu, NMD ATM 2011

13. "Fluid Flow Behavior of LD Converters Using Different" - e Turbulence Model" By T. K. Kundu , S. Pal (presenter and Corresponding Author) ,NMD ATM 2010 Page 77 (2010)

14. "ANN Modeling For Prediction of Phosphorus, Carbon And Temperatures in LD Converter" by T. K. Kundu, S. Pal (presenter and Corresponding Author) ,NMD ATM 2010 Poster Volume, pp. 77 (2010)

Professional Membership

1. Life member in The Indian Institute of Metals (Membership No. LM55478)

2. Life member in Institution of Engineers (Membership No. AM1707232)

Workshop Attended

1st - 5th July 2014	Faculty Development Program in Pedagogy and E-learning Technology **National Institute Of Technology**, Rourkela,India
4th - 5th August 2015	National Workshop on Technology Enabled Learning (TECHEL - 2015) **Organized by A N Khosla Centre for Technology Learning, National Institute of Technology**, Rourkela,India

Team Player and leadership Skill

1. Organized National Conference of Processing Characterization Materials (NCPCM) 2014 conference seminar as a co-convener and treasurer in Metallurgical and Materials Engineering Department of National Institute of Technology Rourkela, India.
2. Organized Research Scholar Day 2011 conference seminar as a convener in Metallurgical and Materials Engineering Department of Indian Institute of Technology Kharagpur, India.

Administrative Responsibilities

•Member of Institute Academic Program Oversight Committee - National Institute of Technology Rourkela (August'2016 – going on)

•Faculty Coordinator - Student Council Centre, National Institute of Technology Rourkela (July'2018 – going on)

•Faculty Advisor for B. Tech students of Metallurgical and Materials Engineering Department, National Institute of Technology Rourkela (July'2014 – going on)

•Worked as an Assistant Warden for a hostel having 1200 boarders in National Institute of Technology Rourkela (July'2015 – June'2017)

•Professor –in –Charge for Departmental Website of Metallurgical and Materials Engineering Department, National Institute of Technology Rourkela (July'2015 – June'2017)

•Member of disciplinary committee of Institute Hall Management Centre - National Institute of Technology Rourkela (August'2016 – June'2017)

•Member of purchase committee of Institute Hall Management Centre - National Institute of Technology Rourkela (August'2015 – June'2016)

Technical Skills

Programming Languages	FORTRAN, C, C++, Matlab,Python
Data Science:	Material Informatics , Machine Learning and Deep Learning
Operating System:	Windows and Linux
Atomistic and Molecular Simulation Packages:	Gaussian 09, Lammps
Computational Fluid Dynamics Package:	Ansys Fluent
Knowledge of Metallurgical Process :	Steel making process, Continuous casting process Microstructure Modeling, Welding Technology, and Failure Analysis

Short Term courses

Date	Topic	Type
18-20 Dec 2020	Conference on Processing and Characterization of Materials (CPCM 2020)	Conference
14-18 June 2021	A Five Day Online AICTE Training and Learning (ATAL) Academic FDP Program On "Cultivating Excellence in Implementation of Computational Science for Scientific and Technological Innovations"	Workshop
22-26 Sep 2020	Molecular Modelling of Materials and Biological Macro Molecules	Workshop
01-05 Nov 2017	5 Day Workshop on Computational Techniques and Mathematical Modelling (CTMM-17) for Academia and Industry	Workshop

Declaration

I declare that all the information of my resume is correct as per my knowledge.

(Dr. Snehanshu Pal)