

CONTACT INFORMATION	<p>Dr. Dhiraj Kumar MAHAJAN Assistant Professor Department of Mechanical Engineering Room No. 114, Satish Dhawan Building, Indian Institute of Technology Ropar, Rupnagar-140001, Punjab, India Tel: +91-1881-23-0110 Mob: +91-7814252244 E-mail: dhiraj.mahajan@iitrpr.ac.in Web: http://www.iitrpr.ac.in/smmee/dhiraj Laboratory: Ropar Mechanics of Materials Laboratory</p>
DATE OF BIRTH	18 th April 1979
SCIENTIFIC RESEARCH INTERESTS	<ul style="list-style-type: none"> • Fracture and fatigue behavior of materials. • Experiment and Simulation-assisted development of polymers for energy and biomedical applications. • Modeling of deformation and failure behavior of polymeric materials using Atomistic and Finite Element Simulations. • Experiment and simulation-based studies of fatigue behavior of steels under hydrogen/aggressive environment. • Atomistic, Dislocation Dynamics and Crystal Plasticity-based modeling of metal plasticity.
ACADEMIC APPOINTMENTS	<p>Assistant Professor December 2013 – Present Department of Mechanical Engineering Indian Institute of Technology Ropar, India</p> <p>Visiting Faculty May 2014 - July 2014 Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr University Bochum, Germany</p> <p>Post Doctoral Research Associate January 2010 - December 2013 Department of Micromechanical and Macroscopic Modelling, ICAMS Ruhr University Bochum, Germany Advisor: Prof. Dr. Alexander Hartmaier</p> <ul style="list-style-type: none"> • Investigations into the fatigue failure of steel under hydrogen environment using coupled framework of hydrogen transport model and crystal plasticity • Study of failure mechanisms of glassy polymer using molecular dynamics simulations • Study of adhesion of polymer coatings on rough surfaces • Study of fatigue crack initiation in metals using new multiscale model
EDUCATION	<p>Indian Institute of Technology, Kanpur, India Ph.D., Department of Mechanical Engineering, December 2010</p> <ul style="list-style-type: none"> • Thesis Topic: <i>Investigations into the deformation behavior of glassy polymers using molecular dynamics</i> • Advisor: Prof. Sumit Basu • Area of Study: Solid Mechanics <p>National Institute of Technology, Warangal, India Master of Technology, Department of Mechanical Engineering, March 2003</p> <ul style="list-style-type: none"> • Thesis Topic: <i>Finite element modeling of isothermal forging process</i>

- Advisor: Prof. P. Bangaru Babu
- Area of Study: Advanced Manufacturing Processes
- Passed with *Distinction*

S.B.S.C.E.T, Ferozepur (**Punjab Technical University**, Jalandhar, India)

Bachelor of Technology, Department of Mechanical Engineering, June 2001

- Area of Study: Production Engineering

TEACHING
EXPERIENCE

Indian Institute of Technology, Ropar, India

Course Instructor

- ME502: Applied Numerical Methods, Jul'19 - Nov'19, 51*
- MEL616: Fracture & Fatigue, Jan'18 - Apr'18, 15*
- GEL102: Materials Science and Engineering, Jul'17 - Nov'17, 68*
- MEL616: Fracture & Fatigue, Jan'17 - Apr'17, 11*
- GEL102: Materials Science and Engineering, Jul'16 - Nov'16, 64*
- MEL616: Fracture & Fatigue, Jan'16 - Apr'16, 13*
- MEL633: Numerical Methods in Mechanical Engineering, Jul'15 - Nov'15, 28*
- IIP201: Core Industry Internship And Colloquium, Jul'15 - Nov'15, 39*
- MEL206: Mechanics of Materials, May'15 - Jul'15, 4*
- MEL203: Manufacturing with Non-Metallic Materials, Jan'15 - Apr'15, 37*
- MEL624: Crystal Plasticity, Jan'15 - Apr'15, 5*
- MEL206: Mechanics of Materials, Jul'14 - Nov'14, 36*
- MEL206: Mechanics of Materials, Jan'14 - Apr'14, 32*

Laboratory Instructor

- GEL102: Workshop Practices (Coordinator), Jul'19 - Nov'19, 162*
- GEL102: Workshop Practices (Coordinator), Jan'19 - Apr'19, 154*
- MEP304: Design Laboratory (Coordinator), Jan'19 - Apr'19, 43*
- ME205: Design Lab-I (Coordinator), Jan'19 - Apr'19, 72*
- GEL102: Workshop Practices (Coordinator), Jul'18 to Nov'18, 137*
- MEP304: Design Laboratory (Coordinator), Jan'18 - Apr'18, 44*
- MEP304: Design Laboratory (Coordinator), Jan'17 - Apr'17, 38*
- MEP304: Design Laboratory (Coordinator), Jan'16 - Apr'16, 38*
- MEP302: Manufacturing Laboratory, Jul'14 to Nov'14, 19*
- MEP304: Design Laboratory, Jan'14 to Apr'14, 21*

*Number of students in class

REFEREED
JOURNAL
PUBLICATIONS

- [15] R. Singh, V. Singh, A. Arora and **D. K. Mahajan**, In-situ investigations of hydrogen influenced crack initiation and propagation under tensile and low cycle fatigue loadings in RPV steel, *Journal of Nuclear Materials*, November 2019, 151912. doi:10.1016/j.jnucmat.2019.151912
- [14] R. Kumar, and **D. K. Mahajan**, Hydrogen Distribution in Metallic Polycrystals with Deformation. *Journal of the Mechanics and Physics of Solids*, 135, February 2020, 103776. doi:10.1016/j.jmps.2019.103776
- [13] R. Singh, and **D. K. Mahajan**, On the transition of fracture toughness in metallic materials with thickness: An atomistic viewpoint. *Computational Materials Science*, Jan 2020, 171, 109268. doi:10.1016/j.commatsci.2019.109268
- [12] V. Singh, R. Singh, K. S. Arora and **D. K. Mahajan**, Hydrogen induced blister cracking and mechanical failure in X65 pipeline steels *International*

Journal of Hydrogen Energy, 44(39), pp. 22039-22049, 2019.
doi:10.1016/j.ijhydene.2019.06.098

- [11] R. Singh, and **D. K. Mahajan**, Role of stress triaxiality on ductile versus brittle fracture in pre-cracked FCC single crystals: An atomistic study. *Modelling and Simulation in Materials Science and Engineering*, May 2019, 27, 055007. doi:10.1088/1361-651X/ab1cb1
- [10] R. Singh, A. Singh, P. K. Singh, and **D. K. Mahajan**, Role of prior austenite grain boundaries in short fatigue crack growth in hydrogen charged RPV steel. *International Journal of Pressure Vessels and Piping*, 171(2019): 242-252, March 2019. doi:10.1016/j.ijpvp.2019.03.004
- [9] H. Singh, J. S. Sidhu, **D. K. Mahajan**, and N. Singh, Carbon Quantum Dots and Rhodamine Based Ratiometric Fluorescent Complex for Recognition of Histidine in Aqueous System. *Materials Chemistry Frontiers*, 3 (2019), 476-483, January 2019. doi:10.1039/C8QM00554K
- [8] **D. K. Mahajan**, and A. Hartmaier. Mechanisms of crazing in glassy polymers revealed by molecular dynamics simulations. *Physical Review E*, 86(2): 021802, August 2012. doi:10.1103/PhysRevE.86.021802
- [7] S. Brinckmann, **D. K. Mahajan**, and A. Hartmaier. A scheme to combine molecular dynamics and dislocation dynamics. *Modelling and Simulation in Materials Science and Engineering*, 20(4): 045001, June 2012. doi:10.1088/0965-0393/20/4/045001
- [6] **D. K. Mahajan**, R. Estevez, and S. Basu. Ageing and rejuvenation in glassy amorphous polymers. *Journal of the Mechanics and Physics of Solids*, 58(10): 1474-1488, October 2010. doi:10.1016/j.jmps.2010.07.015
- [5] **D. K. Mahajan**, and S. Basu. On the simulation of uniaxial, compressive behaviour of amorphous, glassy polymers with Molecular Dynamics. *International Journal Of Applied Mechanics*, 2(3): 515-541, September 2010. doi:10.1142/S1758825110000639
- [4] **D. K. Mahajan**, B. Singh, and S. Basu. Void nucleation and disentanglement in glassy amorphous polymers. *Physical Review E*, 82(1): 011803, July 2010. doi:10.1103/PhysRevE.82.011803
- [3] **D. K. Mahajan**, and S. Basu. Investigations into the applicability of rubber elastic analogy to hardening in glassy polymers. *Modelling and Simulation in Materials Science and Engineering*, 18(2): 025001, March 2010. doi:10.1088/0965-0393/18/2/025001
- [2] M. K. Majumder, S. Ramkumar, **D. K. Mahajan**, and S. Basu. Coarse-graining scheme for simulating uniaxial stress-strain response of glassy polymers through molecular dynamics. *Physical Review E*, 81(1): 011803, January 2010. doi:10.1103/PhysRevE.81.011803
- [1] S. Basu, **D. K. Mahajan**, and E. Van Der Giessen. Micromechanics of the growth of a craze fibril in glassy polymers. *Polymer*, 46(18): 7504-7518, August 2005. doi:10.1016/j.polymer.2005.05.148

BOOK CHAPTER

- [1] R. Singh, and **D. K. Mahajan**, Crystal orientation effect on SIF in single crystals: A study based on coupled framework of XFEM and crystal plasticity model. *Lecture Notes in Mechanical Engineering*, 9789811060014, (2018), pp. 457-471 doi:10.1007/978-981-10-6002-1_37

- [10] R. Singh, A. Singh, P. K. Singh, and **D. K. Mahajan**, Effect of hydrogen on short crack propagation in SA508 Grade 3 Class I low alloy steel under cyclic loading. *Procedia Structural Integrity, Volume 14, 2019, Pages 930-936*
doi:10.1016/j.prostr.2019.07.073
- [9] A. Arora, R. Kumar and **D. K. Mahajan**, In-situ Study of the Effect of Hydrogen on Fatigue Crack Initiation in Polycrystalline Nickel. *Procedia Structural Integrity, Volume 14, 2019, Pages 790-797*
doi:10.1016/j.prostr.2019.07.057
- [8] R. Kumar, D. Meena and **D. K. Mahajan**, Modelling of Fatigue Crack Initiation in Hydrogen Charged Polycrystalline Nickel. *Procedia Structural Integrity 14 (2019) 6686752*
doi:10.1016/j.prostr.2019.05.083
- [7] R. Singh, A. Singh, A. Arora, P. K. Singh, and **D. K. Mahajan**, On the transition of short cracks into long fatigue cracks in reactor pressure vessel steels. *MATEC Web of Conferences 165 (2018) 13001*
doi:10.1051/mateconf/201816513001
- [6] V. Singh, R. Singh, A. Singh, and **D. K. Mahajan**, Tracking hydrogen embrittlement using short fatigue crack behavior of metals. *Procedia Structural Integrity 13 (2018) 14271432*
doi:10.1016/j.prostr.2018.12.296
- [5] V. Singh, and **D. K. Mahajan**, Synergetic effect of hydrogen embrittlement and sensitization on short fatigue crack behavior in AISI 316L steel. In: *Proceedings of Corcon 2018*, 30th Sep-3rd Oct 2018, Jaipur, India.
- [4] **D. K. Mahajan**, R. Swarnkar, Y. Singh, R. Singh, K. S. Arora, M. Shome, and G. Singh, Study of Hydrogen Embrittlement of API X65 & X80 Pipeline Steels using Short Fatigue Cracks. In: *Proceedings of Corcon 2017*, Paper No. CMT25, 17-20 September, Mumbai, India.
- [3] **D. K. Mahajan**, Crystal Plasticity based Modeling of Fatigue Behaviour of Metals under Hydrogen Environment. In: *Proceeding of Multiscale Modeling of Materials and Devices (MMMD-2014)*, October 2014, BARC, Mumbai, India.
- [2] **D. K. Mahajan**, and S. Basu. Parametric study of strain hardening behavior of glassy polymers using molecular simulations. In: *Proceedings of the 22nd ICTAM-2008*, August 2008, Adelaide, Australia.
- [1] **D. K. Mahajan**, and S. Basu. Characterization of deformation behaviour of glassy polymers using molecular dynamics simulations. In: *Proceedings of the 2nd ICCMS-2006*, December 2006, IIT Guwahati, India.

SPONSORED
PROJECTS

S. No.	Title of the Project	Funding Agency	Role (PI/CI)	Status/ Time Frame	Total Cost (Lakhs)
1.	IIT Ropar as National Resource Centre for Manufacturing (Developed 20 hours MOOC Course on Manufacturing with 5 hours video content by Industry leaders in various domains of Manufacturing),	MHRD	PI	Completed/ 2018-2019	14
2.	Study of the Effect of Microstructure on Fatigue Crack Initiation in Nickel under Hydrogen Environment using Coupled Framework of Crystal Plasticity & Hydrogen Transport Model,	DST (Fast track)	PI	Completed/ 2015-2018	29.1
3.	Grant under fund for improvement of S&T infrastructure (FIST). As part of the project implementation group, I am responsible for establishing two facilities in the department i.e. Tensile/Fatigue stage for SEM and EBSD for SEM under this grant.	DST	CI	Ongoing/ 2015-2020	235
4.	Biodegradable Polymeric Stents: From Synthesis of Functionalized Raw Material to its Fabrication using Micro-Injection Moulding Process	DST-Advanced Manufacturing Technology Program 2017	PI	Ongoing/ 2018-2020	47
5.	Design, development, and demonstration of indigenous hydrogen storage and fuel cell system for mobile and stationary applications of 5 kW capacity	IMPRINT (MHRD-MNRE)	Co-PI	Ongoing/ 2017-2020	75 (IIT Ropar) out of 400 (Total)
6.	Development of Compressed Hydrogen-Fuel Cell Integrated System Suitable for Light-Duty Vehicle,	DST	Co-PI	Ongoing/ 2019-2022	2.24 (IIT Ropar) out of 4.6 Crore (Total)
7.	Development of an Effluent Treatment Plant for Hand-tool Industry	Uchchatar Avishkar Yojana (MHRD-DST-MSME)	PI	Ongoing/ 2016-2019	47
8.	Additive Manufacturing & Machine Learning based Development of Indigenous Hydrogen Fuel Cell Stack	DST	PI	approved/to start by December 2019	70
9.	Design and development of a customized elastomeric balloon for a constant air pressure output bio-medical device	COEO Labs, Bangalore	PI	Completed	5.5

ADMINISTRATIVE
SERVICES FOR IIT
ROPAR

- Head, Training & Placement Cell, IIT Ropar from April 2017 onwards. Brought several reforms in the functioning of T&P Cell. Played key role in establishing Career Development & Corporate Relation Centre (CDCRC) at IIT Ropar and to start a B.Tech program with Additional Internship as well as Joint Master thesis with Industry for M.Tech students.
- Coordinator, National Resource Centre for Manufacturing at IIT Ropar from Aug' 2018-Jul'2019 to develop a 40 hour MOOC on Manufacturing. The course is floated on Swayam Platform by GoI and includes extensive inputs by thought leaders from Industry and Academia.
- Organizing Team Member for SAE-BAJA 2018 at IIT Ropar, Jan 17-Mar18.
- Faculty In-charge, Board of Cultural Activities (BOCA), IIT Ropar, Aug'14 - Jun15.
- Established an online teaching feedback mechanism for IIT Ropar, June'14 - Nov14.

AWARDS/
ACHIEVEMENTS

- IIT Ropar student team with Dr. Dhiraj K. Mahajan as advisor won the second prize in HY Contest-2019 organized by Hydrogen Association of India for the project report titled "Modeling the Hydrogen Refueling Station for Heavy Duty Bus Applications".
- International Travel Support Award for attending 13th International Conference on the Mechanical Behavior of Materials held at RIMT, Melbourne, Australia, June 2019.
- In a conference organized by Indian Structural Integrity Society (InSIS) and DMRL naming Structural Integrity Conference and Exhibition 2018 (www.sice2018.in) at Hyderabad from 25th-27th July 2018, two PhD students (Rakesh Kumar and Aman Arora) won the best poster and best presentation awards. (<https://www.sice2018.in/site/conference-awards>)
- IIT Ropar student team with Dr. Dhiraj K. Mahajan as advisor won the Veziroglu Award in the 2017 HY-contest organized by Hydrogen Association of India. (<http://www.hai.org.in/images/past-event.docx>)
- IIT Ropar student team with Dr. Dhiraj K. Mahajan as advisor won the 2015 HY-contest organized by Hydrogen Association of India for design of Hydrogen Refueling Dispensing Station Model. (<http://www.hai.org.in/images/past-event.docx>)
- Best Poster Award at DAE-BRNS Symposium on Multiscale Modeling of Materials and Devices (MMMD-2014) held at Bhabha Atomic Research Center (BARC), Mumbai from October 30 – November 2, 2014.
- Young scientist International Travel Support Award for attending Joint EU-India Grid Tutorial on chemical and material science applications held at ICTP - Trieste, Italy, September 2008.

PROFESSIONAL
EXPERIENCE

Visiting Research Scholar

May 2007 - August 2007

Laboratoire MATEIS-GEMPPM, INSA Lyon, France

Supervisor: Prof. Rafael Estevez

- Numerical simulation of multiple craze generation in Polycarbonate during double notch four point bend (DEN-4PB) test

Research Assistant

Mar 2007 - Nov 2009

Indian Institute of Technology, Kanpur, India

Supervisor: Prof. Sumit Basu

- Development of an experimentally validated simulation scheme for fracture of glassy, amorphous polymers

Industrial Trainee

January 2000 - July 2000

Diesel Loco Modernisation Works, Patiala, India

- Obtained experience in various shop floor activities, jig-fixtured design and production planning and control.

PROFESSIONAL SERVICE

Referee Service

- *Modelling and Simulation in Materials Science and Engineering (MSMSE)*
- *Journal of Elasticity*
- *Journal of Physics: Condensed Matter*
- *Public Library of Science, One (PLOS One)*

CONFERENCE ORGANIZING COMMITTEE

- *Organizing Secretary* for NCRSME-2007: National Conference of Research Scholars in Mechanical Engineering held at IIT Kanpur during 23–24 March 2007 with Prof. P. Venkitanarayanan as Convener and Prof. K. Muralidhar as Patron for the conference.

COMPUTATIONAL SKILLS

Programming

- Fortran, C, C++, Java, Perl, MPI based parallel computing, UNIX shell scripting

Software Development Tools

- Version Control: CVS, SVN
- Documentation System: Doxygen
- Development toolset: Eclipse
- Profiler: Valgrind
- Parallel debugger: Totalview

Numerical Computation Tools

- Matlab: Linear algebra, nonlinear numerical methods, polynomials, statistics, visualization; Maple; Gnuplot
- Solid Mechanics related packages: Abaqus, Ansys, Tecplot
- Atomistic Simulations related packages: LAMMPS, DL-POLY, VMD, IMD, VORO++, Material Studio by Accelrys

Productivity Applications

- \TeX (\LaTeX , \BibTeX , \PSTricks), Vim, most common productivity packages for Windows and Linux platforms

Operating Systems

- Microsoft Windows family, Linux, and other UNIX variants

EXPERIMENTAL SKILLS

Fracture mechanics, Fatigue studies, Mechanical testing of materials under high pressure gaseous environment, Small scale testing of materials under scanning electron microscope using tensile/fatigue stage, Grain boundary engineering using EBSD stage within scanning electron microscope, Scanning electron microscopy, Atomic Force Microscopy, Electroplating, Hydrogen permeation studies using Devanathan-Stachurski cell, Nano-indentation, XRD.

RESEARCH
GUIDANCE

S. No.	Type	Student Name	Research Focus	Time Frame
1.	M.Sc.*	Yashwanth Padharthi	Molecular Modeling of Interface Failure of Stretchable Electronics	Mar'13-Oct'14
2.	PhD	Rajwinder Singh	Investigation into the Short Crack Nucleation and Propagation in Metals under Monotonic and Cyclic Loading	July'14-Oct'19
3.	PhD	Rakesh Kumar	Computational Modeling of the Effect of Microstructure on Fatigue Crack Initiation in Metals under Hydrogen Environment	Jan'15-onwards
4.	M.Tech	Yashpal Singh	Characterization of Hydrogen Embrittlement Using Short Fatigue Crack Behavior of Metals	May'16-July'17
5.	M.Tech	Mukesh Kumar	Design and Material Optimization of Type IV Hydrogen Cylinders using Finite Element-Based Simulation Framework (Co-Supervisor: Dr. Ravi Mohan Prasad)	May'16-July'17
6.	M.Tech	Shovit Sagar	Service Life Prediction of Type III Hydrogen Storage Cylinders (Co-Supervisor: Dr. Srikant S. Padhee)	May'16-July'17
7.	PhD	Navneet Singh	Development and Evaluation of Cavitation-resistant Composite Coatings for Hydro Turbine Steels (Co-Supervisor: Prof. Harpreet Singh)	Jan'16-onwards
8.	PhD	Tushita Rohilla	Experiment and Simulation-assisted development of low-cost hydrocarbon alternatives for perfluorinated Sulfonic Acid (PFSA)-based Polymer Electrolyte Membrane for Hydrogen/Air Fuel Cells	Jul'16-onwards
9.	PhD	Aman Arora	Investigating Fatigue Crack Nucleation in Hydrogen Charged Nickel	Dec'16-onwards
10.	PhD	Harupjit Singh	Development of Polymers/Polymeric composites for Manufacturing of Indigenous Polymeric Stent (Co-Supervisor: Prof. Narinder Singh)	Dec'16-onwards
11.	PhD	Vishal Singh	Experiment and Simulation-assisted Understanding of Hydrogen Embrittlement	Dec'17-onwards
12.	PhD	Mukesh Kumar	Design and Material Optimization of Type IV Hydrogen Storage Tanks for Fuel Cell Driven Vehicles (Co-Supervisor: Dr. Ravi Mohan Prasad)	Dec'17-onwards
13.	MTech	Sandeep Kumar	Effect of Surface Roughness on Fatigue Behavior of Additively Manufactured IN718 Components (Co-Supervisor: Dr. Dheepa Srinivasan)	May'18-onwards
14.	MTech	Mohd. Faisal	Design & Development of Polymeric Stent Using Micro Injection Molding	May'19-onwards
13.	MTech	Akash Bhardwaj	Polymer Electrolyte Membrane Fuel Cell Bipolar Plates Flow Field Simulations AND Development of Fuel Cell Stack	May'19-onwards

* Master of Science in Computational Mechanics at University of Essen-Duisburg, Germany.

CONFERENCE
CONTRIBUTIONS

International

- K. Govind, R. Kumar, D. K. Mahajan, "Effect of microstructure on hydrogen diffusion in metals: A Crystal Plasticity Finite Element Study", 4th International Conference on Hydrogen and Fuel Cell Conference, 6-8 Dec'15, Agra, India. (Talk)
- R. Singh, K. Sharma, P. Ratnam, G. J. Mahajan, S. Kumar, T. Chaudhary,

- V. Khurana, S. S. Padhee, D. K. Mahajan, “Nanoindentation measurements of hydrogen embrittlement in nanocrystalline nickel films”, 4th International Conference on Hydrogen and Fuel Cell Conference, 6-8 Dec’15, Agra, India. (Poster)
- R. Swankar, R. Singh, D. K. Mahajan, “Development of an experimental set-up for determination of dissolved hydrogen and its permeation rate in metals”, 4th International Conference on Hydrogen and Fuel Cell Conference, 6-8 Dec’15, Agra, India. (Poster)
 - V. Gupta, D. K. Mahajan, “Study of the effect of grain boundary type on hydrogen embrittlement of metals using DFT calculations”, 4th International Conference on Hydrogen and Fuel Cell Conference, 6-8 Dec’15, Agra, India. (Poster)
 - V. Goyal, R. Kumar, A. Agarwal, S. S. Padhee, D. K. Mahajan, “Multiphysics simulations of hydrogen diffusion in mechanically loaded metallic lamina”, 4th International Conference on Hydrogen and Fuel Cell Conference, 6-8 Dec’15, Agra, India. (Poster)
 - D. K. Mahajan, “Hydrogen Diffusion Enabled Crystal Plasticity Model: A Computational Framework for Understanding Micro-Structural Effects on Hydrogen Embrittlement of Metals”, International Workshop on Stress Assisted Environmental Damage in Structural Materials, 27th Feb - 2nd Mar’15, IIT Madras, Chennai, India (Invited Talk).
 - D. K. Mahajan, “Surface Roughness Effects on Polymer-Substrate Adhesion: A Molecular Dynamics Study”, RUB Materials Days & International Workshop on Interface-dominated Materials, November 2013, Bochum (Talk).
 - D. K. Mahajan, P. Schwittek, “Coupling H-diffusion and crystal plasticity”, Workshop ”Plasticity and Crack Initiation in Steels”, 14th October 2013, Materials Center Leoben, Austria (Talk).
 - D. K. Mahajan, F. Varnik, A. Hartmaier. “Effect of substrate topography on adhesion properties of polymer coatings”, Sitzung DGM-Fachausschuss Hybride Werkstoffe und Strukturen, October 2013, Kaiserslautern, Germany (Talk).
 - D. K. Mahajan, F. Varnik, A. Hartmaier. “Surface Roughness Effect on Static, Dynamic and Mechanical Properties of Polymers at Interfaces”, 3rd International Conference on Material Modelling (ICMM), September 2013, Warsaw, Poland (Talk).
 - D. K. Mahajan, F. Varnik, A. Hartmaier. “Effect of substrate topography on adhesion properties of polymer coatings”, 7th. International Discussion Meeting on Relaxation in Complex Systems, July 2013, Barcelona (Talk).
 - D. K. Mahajan, A. V. Berezkin, P. U. Biedermann, F. Varnik, A. Hartmaier. “Polymer/Substrate Interfaces: Simulation of Structure, Properties and Behavior”, ICAMS² 2013. May 2013, Bochum (Poster).
 - D. K. Mahajan, F. Varnik, A. Hartmaier. “Effect of surface roughness on cohesive bonding of polymer-solid interfaces“, MMM-2012, October 2012, Biopolis, Singapore (Poster).
 - D. K. Mahajan, S. Brinckmann, A. Hartmaier. “Localization during failure of glassy polymers”, Euromat-2011, September 2011, Montpellier, France (Poster).
 - S.Brinckmann, D. K. Mahajan, C. Begau, A. Hartmaier. “Combined molecular dynamics and dislocation dynamics simulation: A study of dislocation nucleation at crack tips”, Euromat-2011, September 2011, Montpellier, France (Talk).
 - S.Brinckmann, D. K. Mahajan, C. Begau, A. Hartmaier. “The introduction of a concurrent multiscale model for fcc metals”, MMM-2010, October 2010, Freiburg, Germany (Talk).
 - S.Brinckmann, D. K. Mahajan, C. Begau, A. Hartmaier. “The introduction of a concurrent multiscale model for fcc metals“, 18th ECF, Aug-Sep 2010, Dresden, Germany (Talk).
 - D. K. Mahajan, S.Basu. “Parametric study of strain hardening behavior of glassy polymers using molecular simulations”, ICTAM-2008, August 2008, Adelaide, Australia (Talk).
 - D. K. Mahajan, S. Basu. “Characterization of deformation behaviour of glassy

polymers using molecular dynamics simulations”, ICCMS-06, December 2006, IIT Guwahati, India (Talk).

- D. K. Mahajan, S. Basu. “Multiscale modeling of deformation and failure behavior of glassy polymers“, Indo-European Thematic Meeting on Computational Material Science, February 2006, IISc. Bangalore, India (Poster).
- D. K. Mahajan, S. Basu. “Micromechanics of the failure of craze fibril”, Workshop on Mechanical Behavior of Systems at Small Length Scales, January 2004, IISc. Bangalore, India (Poster).

National

- D. K. Mahajan. Modeling of Fatigue Failure of Steels Under Hydrogen Environment. National Conference on Convergence of Science, Engineering & Management in Education and Research, March 2014, Northwest Group of Institutions, Dhudike, Moga, Punjab, India (Invited Talk).

TALKS / DISCUSSION MEETINGS

- [7] Understanding Mechanics of Materials using Stress-Strain Measures that Undergraduate Students Generally Don't Know, 11th February 2015, Department of Mechanical Engineering, Chandigarh Engineering College, Chandigarh, India (Invited talk).
- [6] Understanding Mechanics of Materials using Stress-Strain Measures that Undergraduate Students Generally Don't Know, 11th February 2015, Department of Mechanical Engineering, Rayat-Bahra Institute of Engineering & Bio-Technology, Kharar, India (Invited talk).
- [5] Understanding Mechanics and Physics of Polymeric Materials using Molecular Dynamics Simulations, April 8th 2015, Department of Production Engineering, Punjab Engineering College Univeristy of Technology, Chandigarh, India (Invited talk).
- [4] Crystal Plasticity based Modeling of Fatigue Behavior of Metals Under Hydrogen Environment, 21st August 2014, Department of Mechanical Engineering, Indian Institute of Technology Madras, Chennai, India (Invited Talk).
- [3] Understanding Failure Behavior of Polymers in Bulk and at Rough Substrate Surface Interface Using Molecular Dynamics. 5th November 2013, Department of Material Science, University of Saarland, Germany (Invited Talk).
- [2] Effect of substrate topography on adhesion properties of polymer coatings, 6th August 2013, DLR Cologne, Germany (Discussion Meeting).
- [1] Effect of substrate topography on adhesion properties of polymer coatings, 19th December 2012, TU Eindhoven (TU/e), Netherlands (Discussion Meeting).

TRAINING

- School: Hierarchical Methods for Dynamics in Complex Molecular Systems, 5–9 March 2012, Juelich Supercomputing Centre, Juelich, Germany. (Poster)
- Workshop: Basic tools and techniques for development and maintenance of atomic-scale software, 21–25 June 2010, Z-CAM, Zaragoza, Spain.
- Tutorial: Joint EU-India Grid/CompChem GRID Tutorial on chemical and material science applications, 15–18 September 2008, ICTP - Trieste, ITALY.
- Workshop: Understanding Molecular Simulations, 22–27 January 2007, JNCASR, Bangalore, India.
- Workshop: Polymer Modeling Tools in Material Studio by Accelrys-India, 9–10 August 2006, CSIR-URDIP, Pune, India.
- Short-term summer course: Data Structures and Algorithms, 8 May–10 June, 2006, Department of computer science and Engineering, IIT Kanpur, India.