Gergely Molnár



Birthdate: 27th August 1986

Research Interest

Multi-scale modeling. Mechanical properties of microstructured materials. Computational physics and mechanics. Fragmentation of solids. Numerical modelling of structures. Dynamic properties of solids.

Education

02/2011 - 03/2014	Budapest University of Technology and Economics, Budapest, Hungary
	Ph.D., Mechanics of structural materials, March, 2014
	Thesis: "Multi-scale modelling of structural glass"
09/2009 - 01/2011	M.Sc., Structural and geotechnical engineer, January, 2011
09/2005 - 01/2009	B.Sc., Civil engineer, June, 2009

Employment

10/2018 – Present	INSA Lyon (Lyon, France)
	CINKS researcher (CK), Contacts and Structures Mechanics Laboratory (LaMCoS)
01/2018 - 09/2018	École Centrale de Nantes (Nantes, France) Postdoctoral researcher, Laboratory GeM Advisors: Dr. Julien Réthoré
01/2017 - 12/2017	Univ. Grenoble Alps (Grenoble, France) Postdoctoral researcher, Laboratory 3SR Advisors: Dr. Laurent Orgéas, Prof. David Rodney, Dr. Karim Mazeau
06/2016 - 10/2016	INSA Lyon (Lyon, France) Postdoctoral researcher, LaMCoS Advisor: Prof. Anthony Gravouil
06/2015 - 05/2016	MINES Saint-Étienne (Saint-Étienne, France) Postdoctoral researcher, Materials Sciences and Structures Division Advisors: Prof. Guillaume Kermouche, Dr. Patrick Ganster, Dr. Etienne Barthel
04/2014 - 05/2015	University Claude Bernard Lyon 1 (Lyon, France) Postdoctoral researcher, Institute of Light and Matter Advisor: Prof. Anne Tanguy

Research Experience

École centrale de Nantes, Laboratory GeM

Advisor: Dr. Julien Réthoré Project: Simulation of dynamic fracture propagation in Penrose tiling

- The project is dedicated to simulate the fragmentation of 2D structures based on Penrose tiling.
- Using coarse-graining techniques on discrete beam models, a constitutive model based on Cosserat theory is created.
- At the continuum scale, to simulate dynamic fracture, a new enriched phase-field element is developed.

Univ. Grenoble Alps, Laboratory of Sols, Solids, Structures and Risks (3SR Lab) Advisor: Dr. Laurent Orgéas, Prof. David Rodney, Prof. Pierre Dumont, Dr. Karim Mazeau Project: *Multi-scale numerical simulation of nanofibrils of cellulose*

- The project is dedicated to deduce the gel-like rheology of concentrated NFC suspensions from the nanostructure and the mechanics of nanofibrils of cellulose
- Using atomic scale simulations, the elementary elasto-plastic properties of cellulose crystals are studied.
- Based on Kirchhoff's beam theory a hybrid discrete element method is used to determine the yield surface of these gel-like materials.
- 1 paper published.

INSA Lyon, Contact and Structure Mechanics Laboratory (LaMCoS) Advisor: Prof. Anthony Gravouil, Dr. Nawfal Blal Project: *Numerical simulation of fracture in brittle materials*

- Present work deals with the implementation of a coupled displacement and **phase field** finite element. The material parameters of the phase field method are identified by **Molecular Dynamics** (MD).
- Additionally I was working with homogenization techniques to couple the mechanical response of atomic medium and continuum methods.
- 1 paper published.

MINES Saint-Étienne, Materials Science and Mechanical Engineering Advisor: Prof. Guillaume Kermouche, Dr. Patrick Ganster, Dr. Etienne Barthel Project: *Finite element implementation of user defined constitutive models*

- The project dealt with the **Finite Element** (FE) implementation of the user defined constitutive model developed using atomic scale simulations.
- The results were compared with real life microscopic experiments such as micro-pillar compression, micro-indentation
- 2 papers published.

University Claude Bernard Lyon 1, Institute of Light and Matter (ILM)

Advisor: Prof. Anne Tanguy, Dr. Patrick Ganster

Project: Material model development using atomic scale simulations

- Work involved quasi static deformation of sodium silicate samples using MD and Monte Carlo simulations. Both global and local stress, strain fields and stiffness properties were calculated using **coarse graining** techniques.
- Using the microscopic results a continuum based **material model** was developed for sodium silicate.
- 3 papers published.

Budapest University of Technology and Economics, Department of Structural Mechanics Advisor: Prof. Imre Bojtár, Dr. János Török

Project: Determining the strength of structural glass using multi-scale methods

- The work involved the mechanical deformation of atomic systems, the stress analysis of structural glass plates caused by **manufacturing defects** and the both theoretical and experimental analysis of **crack propagation** in **tempered glass**.
- It has included the use of the following simulation techniques: MD, FE and Hybrid Discrete Element Method (HDEM).
- And the following experimental applications: Atomic Force Microscopy (AFM), Micro CT, Scattered Light Polariscope (SCALP) and High Speed Recording.
- Published a total number of 7 papers.

Awards

- Best foreign Postdoctoral researcher in Lyon (by AAUL), 2016 (Multiscale mechanical modelling of sodium silicate glasses)
- Conference grant for Early Stage Researchers (by COST), 2014 (Rate dependent elastic response of modelled soda-lime- silica)
- Itasca Education Partnership Mentorship Program (by Itasca Inc.), 2013 (Post-brakeage behavior of laminated glass panels)
- 1th prize of the National Conference of Scientific Students' Associations (OTDK), 2011 (Numerical stability and critical time step evaluation of explicit solvers)
- Diploma Award Competition of the Hungarian Engineering Chamber, 2009 (Glass roof reconstruction for the central building of BUTE)

Conference presentations

- 10th European Solid Mechanics Conference, 2018, Bologna, Italy (invited)
- GDR MéPhy (Mécanique et Physique des Sytèmes Complexes), 2017, Paris, France
- The 4th International Cellulose Conference, 2017, Fukuoka, Japan
- International Symposium on Defects and Material Mechanics , 2017, Lyon, France
- Challenging Glass 5, 2016, Ghent, Belgium (invited)
- MRS 2015 Fall Meeting & Exhibit, Boston, USA
- CFM 2015 French Congress on Mechanics, 2015, Lyon, France
- GDR CNRS 3532 MODMAT Modeling of Materials, 2015, Lyon, France
- Challenging Glass 4 & COST Action TU0905 Final Conference, 2014, Lausanne, Switzerland

- Third Conference on Particle-Based Methods, 2013, Stuttgart, Germany
- COST Action TU0905, Mid-term Conference on Structural Glass, 2013, Poreč, Croatia
- 8th European Solid Mechanics Conference, 2012, Graz, Austria

Invited seminars and workshops

- 3SR, UGA, Grenoble, France, 2017 (Numerical modeling of brittle fracture using the phase-field method)
- PMMH, ESPCI, Paris, France, 2107
 - (Multiscale methods for the analysis of plastic deformation of amorphous materials)
 - GeM, ECN, Nantes, France, 2017

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- (How to determine the resistance of amorphous systems from atomic scale simulations)
- 3SR, UGA, Grenoble, France, 2017
 - (Multi-scale modeling of silicate glasses from the atomic level to continuum)
- MATEIS, INSA, Lyon, France, 2017 (Multi-scale analysis of the strength of silicate glasses)
- LaMCoS, INSA, Lyon, France, 2016 (Plastic material model development for amorphous silica)
- MultiScale Material Science for Energy and Environment, MIT, Boston, USA, 2015 (Multiscale mechanical analysis of sodium silicate glasses)
- Solid Mechanics Laboratory, École Polytechnique, Paris, France, 2015 (Atomic scale plasticity and plastic event formation in sodium silicates)

Research related activities

- Editorial board member of Glass Structures & Engineering (Springer)
- Referee for Acta Materialia (Elsevier) and Periodica Polytechnica Civil Engineering (BUTE)
- Member of TUD COST Action TU0905 Structural Glass, 2012-2014

Teaching Experience

 02/2011 - 03/2014 Teaching Assistant, BUTE, Budapest, Hungary Statics, strength of materials, advanced mechanics and dynamics
02/2015 - 08/1025 MSc Thesis supervisor, MINES, Saint Etienne, France (Lucas Kurth)

Personal pages

Personal webpage: www.molnar-research.com Google Scholar: https://scholar.google.fr/citations?user=KWldOG8AAAAJ&hl=en Scopus: https://www.scopus.com/authid/detail.uri?authorId=55324621300 WoS: http://www.researcherid.com/rid/N-9034-2016 LinkedIN: https://www.linkedin.com/in/gergely-molnár-162a4348/?trk=hp-identity-name

List of publications

Papers in Refereed Journals

- 1. **G. Molnár**, D. Rodney, P. Dumont, F. Martoïa, Y. Nishiyama, K. Mazeau, L. Orgéas, Cellulose crystals plastify by localized shear, P. Nat. Acad. Sci. USA 115 (28) 7260-7265, 2018.
- G. Molnár, G. Kermouche, E. Barthel, Plastic response of amorphous silicates, from atomistic simulations to experiments – A general constitutive relation, Mechanics of Materials, 114 pp. 1-8, 2017.
- 3. **G. Molnár**, P. Ganster, A. Tanguy, Effect of composition and pressure on the shear strength of sodium silicate glasses: An atomic scale simulation study, *Physical Review E*, 95, 043001, 2017.
- 4. **G. Molnár**, A. Gravouil, 2D and 3D Abaqus implementation of a robust staggered phase-field solution for modeling brittle fracture, *Finite Elements in Analysis and Design*, 130 pp. 27-38, 2017.
- 5. **G. Molnár**, P. Ganster, A. Tanguy, E. Barthel, G. Kermouche, Densification dependent yield criteria for sodium silicate glasses An atomistic simulation approach, *Acta Materialia*, 111 pp. 129-137, 2016.
- 6. G. Molnár, P. Ganster, A. Tanguy, J. Török, G. Kermouche, Transition from ductile to brittle failure of sodium silicate glasses: a numerical study *MRS Advances*, 1(24) pp. 1797-1802, 2016.
- 7. **G. Molnár**, P. Ganster, J. Török, A. Tanguy, Sodium effect on static mechanical behavior of MD-modeled sodium silicate glasses, *Journal of Non-Crystalline Solids*, 440 pp. 12-25, 2016.
- 8. **G. Molnár**, M. Ferentzi, Z. Weltsch, G. Szebényi, L. Borbás, I. Bojtár, Fragmentation of wedge loaded tempered structural glass, *Glass Structures & Engineering*, pp 1-10, 2016.
- 9. G. Molnár, I. Bojtár, The effects of the manufacturing inhomogeneities on strength properties of float glass. *Mechanics of Materials*, 59 pp. 1-13, 2013.
- G. Molnár, L.G. Vigh, Gy. Stocker, L. Dunai, Finite Element Analysis of Laminated Structural Glass Plates With Polyvinyl Butyral (PVB) Interlayer. *Periodica Polytechnica Civil Engineering*, 56(1) pp. 35-42, 2012.
- 11. **G. Molnár**, L.M. Molnár, I. Bojtár, Preparing a comprehensive analysis of the mechanical classification of structural glass, *Materials Engineering*, 19 pp. 71-81, 2012.
- 12. G. Molnár, L.M. Molnár, I. Bojtár, Multi-Scale Analysis of Structural Glass, Imaging of The Mesostructure, *Journal of Material Testers*, 21(3-4) pp. 1-14, 2012.
- 13. G. Molnár, I. Bojtár, Solution of 1D Finite Element Problems With Explicit Time Integration, *Architectonics and Architecture*, 40(1) pp. 5-32, 2012. *(in Hungarian)*
- 14. G. Molnár, L.G. Vigh, Gy. Stocker, Load bearing capacity of laminated glass, *Magyar Építőipar*, 62(1) pp. 17-23, 2012. (*in Hungarian*)

Proceedings of Refereed Conferences

- 15. G. Molnár, I. Bojtár, J. Török, Microscopic scale Simulations of Soda-Lime-Silica Using Molecular Dynamics. Proc. of PARTICLES 2013, Stuttgart, Germany, pp. 1-7, 2013. (ISBN: 978-84-941531-8-1)
- 16. **G. Molnár**, Discussion on the micro-mechanics of structural glass. *Proceedings of the 2nd Conference of Junior Researchers in Civil Engineering, Budapest, Hungary* pp. 1-4, 2013.
- G. Molnár, I. Bojtár, J.H. Nielsen, Ongoing model development analyzing glass fracture. COST Action TU0905 Mid-term Conference on Structural Glass. Porec, Croatia, pp. 197-204, 2013. (ISBN: 978-1-138-00044-5)

- M. Vanderbroek, J. Belis, C. Louter, G. Molnár, Ratio of mirror zone depth to flaw depth after failure of glass beams. *COST Action TU0905 Mid-term Conference on Structural Glass. Porec, Croatia*, pp. 235-241, 2013. (ISBN: 978-1-138-00044-5)
- G. Molnár, Mesoscale defects of Structural Glass. Proceedings of the Conference of Junior Researchers in Civil Engineering, Budapest, Hungary, pp. 135-139, 2012. (ISBN: 978-963-313-061-2)
- G. Molnár, Effect of the Mesoscale Defects on the Strength Properties of Structural Glass, *COST Training School "Structural Glass" Student Colloquium, Ghent, Belgium*, pp. 15-18. 2012. (ISBN: 978-94-6197-029-9)
- 21. G. Molnár, Experimental and Numerical Examination of Laterally Loaded Laminated Glass, 28th Danubia-Adria-Symposium on Advances in Experimental Mechanics, Siófok, Hungary, pp. 263-264. 2011. (ISBN: 978-963-9058-32-3)
- 22. G. Molnár, The Mechanical Behaviour of Laterally Loaded Laminated Structural Glass, 11th Hungarian Conference on Theoretical and Applied Mechanics, Miskolc, Hungary, pp. 1-6. 2011. (ISBN: 978-963-661-975-6)