# Gergely Molnár 



Birthdate: $27^{\text {th }}$ 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 <br> Thesis: "Multi-scale modelling of structural glass" |
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| 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) <br> CNRS researcher (CR), 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) <br> Postdoctoral researcher, Laboratory 3SR <br> Advisors: Dr. Laurent Orgéas, Prof. David Rodney, Dr. Karim Mazeau |
| 06/2016-10/2016 | INSA Lyon (Lyon, France) <br> Postdoctoral researcher, LaMCoS <br> Advisor: Prof. Anthony Gravouil |
| 06/2015-05/2016 | MINES Saint-Étienne (Saint-Étienne, France) <br> 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
(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.
2. G. Molnár, G. Kermouche, E. Barthel, Plastic response of amorphous silicates, from atomistic simulations to experiments - A general constitutive relation, Mechanics of Materials, $114 \mathrm{pp} .1-$ 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.
10. 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 Épitőipar, 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.
17. 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)
18. 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)
19. 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)
20. 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)
