Extended Curriculum Vitae Nele Moelans

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Personalia

http://nele.studentenweb.org
https://www.mtm.kuleuven.be/Onderzoek/Semper/SolMicS
https://www.researchgate.net/profile/Nele_Moelans
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Name: Nele Moelans
Date of birth: July 12, 1977
Place of Birth: Leuven
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Job experience and education

- October 2015 - : **Associate professor** at KU Leuven (BOF-KU Leuven Research professor), Department of Materials Engineering
  - **Research expertise and interests:** phase-field modelling of microstructure evolution, calculation of multi-component phase diagrams (CALPHAD), equilibrium and non-equilibrium thermodynamics, diffusion (couple) experiments and modeling, phase transformations, interfaces, grain growth, lead-free soldering, thermodynamics and kinetic modeling of nanowire growth, HEA (or multi-principle alloys), materials informatics, ICME
  - **Teaching:**

  - Computational Thermodynamics in Materials Design, master in Materials Science, KU Leuven (B-KUL-H02V3A)
  - Materials Modeling and Simulation Techniques, Master in Materials Science, KU Leuven (H0S49A)
  - Structuurgenese van materialen (Structure formation of materials), Bachelor in Materials Science, KU Leuven (B-KUL-H01I8A)
  - Athens course at KU Leuven on "Small Scale Modeling Techniques for Materials" (Nov. 2015, Nov. 2016)

- October 2010 - September 2015: **Assistant professor** at KU Leuven (BOF-KU Leuven Research professor), Department of Materials Engineering.

- October 2006 - September 2010: **Postdoctoral Fellow of the Research Foundation - Flanders (FWO-Vlaanderen)** at Department of Materials Engineering, KU Leuven, Belgium

- September 2008 - August 2009: **Postdoc at Lawrence Livermore National Laboratory (LLNL)**, Condensed Matter & Materials Division, California, USA.

- October 2002 - September 2006: **Doctoral student in Engineering granted by the Institute for the Promotion of Innovation by Science and Technology in Flanders (IWT-Flanders)** affiliated with Department of Materials Engineering, KU Leuven

  - Doctorate obtained on May 19, 2006 with *Summa cum laude with the congratulations of the Examination Board* (only awarded in exceptional circumstances, at most 5% of the doctorates in engineering at KU Leuven)
  - Topic: Phase-field simulations of grain growth in materials containing second-phase particles; Abstract and thesis text: http://hdl.handle.net/1979/309

- September 1997 - June 2002: **Master of Science in Materials Engineering** at Department of Materials Engineering, KU Leuven

  - M.S. degree with *Summa cum laude*
  - Master thesis: Calculation of phase diagrams for lead-free solder alloys based on Bi-In-Sn-Zn; Abstract (English and Dutch) and thesis text (Dutch only) on http://nele.studentenweb.org/docs/thesis.pdf

- Summer 2001: **Summer training at R&D Umicore**, Olen, Belgium

  - Topic: Ex-situ pO_2-measurements of non-ferrous slags

- Summer 2000: **Summer training at IMEC (Interuniversity MicroElectronics Center)**, Leuven, Belgium

  - Topic: MOKE (Magneto Optical Kerr Effect) - measurements of soft magnetic materials

- 1996 - 1997: Preparatory year on mathematics, KU Leuven

- 1995 - 1996: Higher education for dance and dance pedagogy (Hoger Instituut voor Dans en Danspedagogie), Lier, Antwerp, Belgium

- 1989 - 1995: High school, Paridaens Instituut, Leuven, Option Greek-Latin

Memberships, commissions, responsibilities

- Member high performance computing steering committee, KU Leuven (since 2014)
- Member User Committee Flemish Supercomputer Centre (VSC) (member : 2014-2017) (substitute member 2017-2020)
- Spokes person KU Leuven in the SRN (Scientific Research Network) on Computational modeling for materials (sponsored by FWO-Flanders) (2010 - 2014 and 2014-1018)
- Reviewer national and international project proposals (KU Leuven, SNSF, NSERC, NCN-Poland, ANR . . .)
- Reviewer journal papers for various journals in the field of materials science, alloy development and characterization and computational materials science (such as Acta Mater., Comp. Mater. Sci, Phys. Rev. B/E/Lett., MSMSE, CALPHAD, Scripta Mater.,Scientific reports . . .)
- Examiner PhDs at and outside KU Leuven
- External evaluator professor candidates
- Guest editor of 2 special issues of an international journal on multi-scale modeling
  - "Multi-Scale Modeling of Moving Interfaces in Materials". Mathematics and Computers in Simulation (Elsevier), 80 (7), 1359-1360, March 2010.
  - "Multiscale Simulation of Heterogeneous Materials and Coupling of Thermodynamic Models". Computational Material Science (Elsevier), Vol 66, January 2013.
- Management Committee member and working group leader in COST MP0602 (2007 - 2011)
- Member of COST 531 Lead-free solder materials and COST 535 Thermodynamics of alloyed aluminides (2005-2007)
- Member (2000-2003) and secretary (2003-2006) of the P.O.C.-commission for Materials Engineering at KU Leuven

Publication record

- Unique research identifier (ORCID): `orcid.org/0000-0003-3361-2954`
- ResearchID: `http://www.researcherid.com/rid/A-3165-2013`
- Google scholar: `https://scholar.google.be/citations?hl=nl&user=x_x0MmQAAAAJ`
- >60 publications in internationally reviewed journals
- 4 contributions in books
- >25 conference proceedings
- >80 conference presentations of which >25 invited
- h-index: 14 (Scopus); 17 (Googlescholar)
- Total citations: >1100 in Scopus; >1500 in Googlescholar

Grants and honors

- ERC Starting Grant 2016 "Unravelling interdiffusion effects at material interfaces – Learning from tensors of microstructure evolution simulations (INTERDIFFUSION)" (1.5 M€)
- Acta Materialia Outstanding Reviewer in 2016 (200 $).
  (https://www.journals.elsevier.com/acta-materialia/news/acta-journals-outstanding-reviewers-in-2016-acta-materialia)
- *Highly cited* paper in WebofScience. "An introduction to phase-field modeling of microstructure evolution", N. Moelans, B. Blanpain, P. Wollants. CALPHAD – Computer Coupling of Phase Diagrams and Thermochemistry, 32, 268-294 (2008)
- Marie Sklodowska-Curie Actions Seal of Excellence (25 April 2017). (Researcher: Hong Liu. Supervisor: Nele Moelans)
- CALPHAD poster award 2013. Best poster presented at CALPHAD XLII Conference, San Sebastian, Spain, 2013: "New Quantitative Phase-Field Model for Elastically Inhomogeneous Systems" A. Durga, P. Wollants, N. Moelans. (300 $)
- Discussion leader, Gordon Research Conference Physical Metallurgy: Evolution of Metals Structures: Modeling, Characterization and Design. Stonehill College, Easton, MA, USA, July 31- Aug 5, 2011.
- Research paper in top 10 of most downloaded papers in April to June 2011 of CALPHAD – Computer Coupling of Phase Diagrams and Thermochemistry: "Calculation of phase equilibria for an alloy nanoparticle in contact with a solid nanowire", Y. Eichhammer, M. Heyns, N. Moelans.
- STT grant (Foundation for applied Thermodynamics, KTH, Sweden) to attend the Winter School on Fundamentals of Thermodynamic Modeling of Materials, Saclay, France, Nov 15-19, 2010.
- Highlight lecture at Euromat 2009, Glasgow, UK: "Phase field simulations of recrystallization in Al-Mn alloys containing Al6Mn precipitates"
- Ph. D. frontier research poster award at the Gordon Research Conference on High Temperature Materials, Processes and diagnostics, Colby College, Waterville, ME, July 16-21 2006: "3D Phase field simulations of grain growth in thin films: pinning effect of second-phase particles and thermal grooving"
- PhD degree obtained with *Summa cum laude with the congratulations of the Examination Board* (only awarded in exceptional circumstances, at most 5% of the doctorates in engineering at KULeuven)
- Postdoctoral fellowship of FWO, 2006-2010
- 1-year mobility grant FWO 2008-2009
- Doctoral grant of IWT-Flanders, 2002-2006

Organization conferences, workshops, seminars

- Co-organiser symposium Advanced modelling techniques: phase field and diffuse interface approaches at 16th European Mechanics of Materials Conference, EMMC16, March 16-18, 2018, Nantes (France).
- Session organiser Multiscale modelling of microstructure evolution and materials mechanics at IWCMM - 27th International Workshop on Computational Mechanics of Materials, Belgium (Leuven), 20-22 September 2017.
- Res Metallica 2017, Multi-scale modeling of materials, KU Leuven, Leuven, Belgium, May 17, 2017.
- Co-organiser symposium Microstructure Evolution in Materials: Mechanisms, Properties, Manufacture at Multiscale Materials Modelling (MMM), Oct 9-14, 2016, Dijon, France.
- Res Metallica 2016, Looking deep into materials, KU Leuven, Leuven, Belgium, May 11, 2016.
- Member scientific committee of the Third International Symposium on Phase Field Method –PFM 2014, State College, Pennsylvania, August 26-29, 2014 (organised by I. Steinbach and L.-Q. Chen)
- Local organisation of Computational Thermodynamics and Kinetics Seminar (ThermoCalc user meeting), Leuven, April 23-24, 2013.
- Workshop on Mesoscale and continuum scale modeling of materials defects, Nov. 13-16 2012. Organizers: V. Shenoy, N. Ghoniem, David Kinderlehrer, Nele Moelans, John Lowengrub. Part of a series of workshops on modeling of defects in materials organized at IPAM, Institute for Pure and Applied Mathematics, UCLA, California, USA.
- Organizer of the workshop Multiscale Simulation of Heterogeneous Materials and Coupling of Thermodynamic Models, 12-14 January, 2011, K.U. Leuven, Belgium, together with G. Samaey
- Co-organiser symposium on Thermodynamics and kinetics: modelling of phase diagrams and microstructure evolution (D34) Euromat 2011, Montpellier, France, 12-15 September (Organiser: Hans Seifert, Co-organisers: Rainer Schmid-Fetzer, Nele Moelans)
- Member international advisory board of TOFA 2010, Discussion Meeting on Thermodynamics OF Alloys, Porto, Portugal, 12-17 September 2010
- Organizer COST MP0602 Working Group 3 meeting on Study of the Interfacial Reactions in Lead-Free Solder Joints for High Temperature Applications, K.U. Leuven, Belgium, January 6-7, 2010.
- Member scientific committee of Second Decennial Symposium on Phase-Field Modelling in Materials Science, Aachen, September 2009 (chairmen I. Steinbach and L.-Q. Chen)
- Organizer of the workshop Multi-Scale Modeling of Moving Interfaces in Materials, 2-4 July, 2008, K.U. Leuven, Belgium, with G. Samaey

- Organizer of the symposium Towards Realistic Three-Dimensional Phase-Field Simulations for the Evolution of Polycrystalline Structures on the SIAM - conference on Mathematical Aspects of Materials Science, Philadelphia, May 2008

PhD students

Completed

- J. Heulens (M.S. degree in Materials Engineering, K.U.Leuven), Isothermal crystallization of metallurgical slags: Phase field simulations combined with in situ experiments, October 2007 - December 2011, promotors: N. Moelans, B. Blanpain, granted by IWT-Vlaanderen.
- Y. Eichhammer (M.S. degree in Engineering from Ecole Centrale de Lille), Thermodynamic and Kinetic Description of Nanowires and Nanowire growth, promotoren: N. Moelans and M. Heyns, November 2007 - February 2012, IMEC funding for fundamental doctoral research.
- A. Durga (B.S. degree in Metallurgy and Materials Engineering, Indian Institute of Technology Madras, IIT Madras), Development of an elastoplastic phase-field model for multi-phase systems, October 2010 - March 2015, promotors: N. Moelans and P. Wollants, financed by OT/07/040 and CREA/12/012 (KU Leuven project funding).
- H. Ravash (M.S. degree in Materials Science from Chalmers University, Sweden), 3D phase-field simulations of sintering and coarsening in polycrystalline multi-phase materials, September 2010 - December 2014, promotors: N. Moelans, J. Vleugels. Financed by SIM project SOPPOM, SBO absCIGS.
- Yuanyuan Guan (M.S. degree in Materials Engineering, KU Leuven), Development of a method to determine the solubility ranges of intermetallic compounds in metal-metal connections, September 2011 - November 2015, Promotor: N. Moelans, financed by OT/07/040 and CREA/12/012 (KU Leuven project funding).
- Evelien De Wilde (M.S. degree in Chemistry, U Ghent), Methodology Development and Experimental Determination of the Origin of Sticking Copper Droplets in Pyrometallurgical Slags, September 2011 - December 2015. Promotors: Kim Verbeken (Ughent), N. Moelans. Financed by IWT-Baekeland with industrial promotor Umicore.
- Jingjing Liu (M.S. degree Materials Science and Engineering,Zhejiang University, China), In-situ observation and phase-field simulation of crystallization and dissolution phenomena in CaO-Al2O3-SiO2 slags, October 2011 -August 2016. Promotors: N. Moelans and M. Guo. Financed by a CSC grant (China Scholarship Council).
- Andrea Isabel Gil Santos (M.S degree in material physics from Complutense University of Madrid (UCM); Master in Laser Technology at Polytechnic University of Madrid (UPM)), Phase diagram assessment and alloy characterization of ternary Mg rich Mg-Si-Ca and Mg-Si-Sr alloys for biomedical applications, Sept 2012 - May 2017, Promotors: O. Vanderbiest, N. Moelans. Financed by the Marie Curie International training network MagnIM.
- Inge Bellemans (M.S. degree in Engineering Science, Materials, U Ghent), Metal droplet entrainment by solid particles in slags: A combined phase field – experimental approach, Oct

2013-May 2017. Promotors : Kim Verbeken (U Ghent), Nele Moelans. Financed by FWO PhD fellowship.

- Nabi Nabioli (M.S degree in Microtechnology and nanoscience Chalmers University of Technology, Gothenburg, Sweden), Processing induced changes of mechanical stresses in and near Cu Through Silicon Vias (TSVs): a finite element modelling study, December 2011 - December 14, 2017, Promotors: I. Dewolf, N. Moelans. Financed by Imec, Leuven.

Ongoing

- Athina Puype (M.S. degree in Engineering Science, Materials, U Ghent), Development of improved ferritic/martensitic creep-resistant steels for nuclear energy, start Sept 1, 2014. Promotors : Jilts Sietsma, Nele Moelans, financed by OCAS+SCK-CEN.
- Lin Hou (M.S. degree in Materials Engineering, KU Leuven), Miniaturization of Solder Balls for 3D Silicon Chip Interconnection, start October 1, 2015. Promoters: I. Dewolf, N. Moelans. Financed at Imec, Leuven.
- Yuri Coutinho (B.S. degree Mechanical Engineering Rio de Janeiro State University, M.S. degree Materials Science and Engineering, Alfred University), Phase-field modeling and quantification of microstructure evolution at multi-component material joints, start May 1, 2017. Promoters: N. Moelans, L. Delathauwer, financed by ERC-StG-2016 INTERDIFFUSION (n° 714754).
- Sourav Chatterjee (M.S. Materials Science IIT Bombay), Phase-field modeling of microstructure evolution in mechanically loaded material joints, start Aug 1, 2017. Promoters: N. Moelans, financed by ERC-StG-2016 INTERDIFFUSION (n° 714754).
- V. Yadav (M.S. degree in Metallurgy and Materials Engineering from Indian Institute of Technology Bombay, IIT Bombay), Modeling and simulation of grain growth and coarsening in polycrystalline single and two-phase materials. Promotors: P. Wollants, N. Moelans. Financed from FWO-project G.0362.09N.

Postdocs

- Irina Nizovtseva, visiting postdoc affiliated with Department of Physics and Astronomy, Friedrich Schiller University of Jena, Germany. Research project: Development of rapid solidification models for multi-phase systems. Collaboration funded through Alexander Humbold Foundation, Oct 2017-.
- Hong Liu, PhD from Monash University in 2015. FWO Pegasus Marie Curie fellowship March 2017-Febr 2020. Research project: Phase-field modeling and simulation of twinning in materials with hexagonal symmetry.
- Hou Yanhui, Wuhan University of Technology, China. March - May 2011 funded by National Natural Science Foundation of China, October 2011 - March 2012, funded by EXPERTS Scholarship (Erasmus Mundus, Europe). Research topic: ab initio calculations of surface and interfacial properties of precipitates in Al-Cu-Mg-(Ag) alloys.

- Yuan Yuan (PhD in 2012 at Central South University, China). Research project: Integrated approach for predicting the microstructure evolution of multi-component joints based on combinatorial key-experiments, phase diagram calculation and microstructure simulation. Financed as FWO Pegasus Marie Curie postdoctoral fellow, Oct 2012 - Sept 2016.
- Kunok Chang (PhD in 2011 at Penn. State University, USA). Research topic: Phase-field simulations of grain growth and the effect of texture and pinning precipitates on grain growth. Oct 2012-Aug 2013. Financed from CREA/12/012 (KU Leuven funding).
- Liesbeth Vanherpe (PhD in 2010 at KU Leuven, Department of Computer Science). Research topic: Bounding box sparse data structure framework for phase field simulations of grain growth in polycrystalline materials. Sept-Oct 2010. Financed from OT/07/040 (KU Leuven funding).