

Curriculum Vitae Nele Moelans

Personalia

Name: Nele Moelans

Date of birth: July 12, 1977

Place of Birth: Leuven

Nationality: Belgian

Current work address (until August 31, 2009): Physical Division, Lawrence Livermore National Laboratories (LLNL), 7000 East Avenue, Livermore, CA 94550, USA

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Education and job experience

- **October 2006 - September 2009:** Postdoctoral Fellow of the Research Foundation - Flanders (FWO-Vlaanderen)
 - Connected with the department of Metallurgy and Materials Engineering, Katholieke Universiteit Leuven
 - Currently working at Lawrence Livermore National Laboratories (LLNL), California, USA
 - Main research interests: phase-field modelling, phase diagrams, thermodynamic modelling, grain growth, lead-free soldering, thermodynamics for small (nano) systems
 - Teaching: 'Chemical materials science II: Thermodynamic modelling and the calculation of phase diagrams' (Master in material science and engineering, K.U.Leuven)
 - Supervision of doctoral, master and bachelor theses in materials engineering and computer science

- **October 2002 - September 2006:** Ph.D. in Engineering (Doctor in de Ingenieurswetenschappen), granted by IWT-Vlaanderen
 - Department of Metallurgy and Materials Engineering, Katholieke Universiteit Leuven
 - Topic: Phase-field simulations of grain growth in materials containing second-phase particles

- Ph.D.-degree obtained on May 19, 2006 with 'Summa cum laude with congratulations of the Board of Examiners'
- Teaching: Exercises thermodynamics (Bachelor in engineering)
- Supervision of master theses in materials engineering and computer science
- Secretary of the POC for materials science (Commission for permanent evaluation of the curriculum and courses)
- **September 1997 - June 2002:** Master of Science in Materials Engineering (Burgerlijk materi-aalkundig ingenieur)
 - Department of Metallurgy and Materials Engineering, Katholieke Universiteit Leuven
 - Master thesis on 'Calculation of phase diagrams for lead-free solder alloys based on Bi-In-Sn-Zn'
 - Graduated with 'Summa cum laude'
 - Summer training at R&D, Umicore, Olen (Summer 2001)
 - * Topic : Ex-situ pO_2 -measurements of non-ferrous slags
 - Summer training at R&D, IMEC, Leuven (Summer 2000)
 - * Topic : MOKE (Magneto Optical Kerr Effect) - measurements of soft magnetic materials
 - Member of the POC for material science (Commission for permanent evaluation of the curriculum and courses)
- **1996 - 1997:** Preparatory year on mathematics (Vorbereidend Jaar Wiskunde), Katholieke Universiteit Leuven
- **1995 - 1996:** Classical dance, Hoger Instituut voor Dans en Danspedagogie, Lier
- **1989 - 1995:** High school
 - Paridaens Instituut, Leuven
 - Option Greek-Latin

Main research interests

- Phase field modelling and numerical simulation of microstructure evolution in polycrystalline, multi-component and multi-phase systems: model formulation and implementation.
 - Grain growth and recrystallization in the presence of a finely-dispersed second-phase (Zener pinning), grain growth in systems with anisotropic grain boundary properties (abnormal grain growth, movement of subboundaries), grain growth and thermal grooving in thin films
 - Growth and coarsening of the intermetallic layer and precipitates in lead-free solder joints
 - * Coupling of the phase-field theory with the CALPHAD-methodology for the calculation of phase equilibria in multi-component alloys
 - * Effect of diffusion and transformation and thermal strains

- Coupling of the phase-field method for microstructure evolution simulations with simulation techniques on other length and time scales in multi-scale approaches
- Phase diagram determination and thermodynamic characterization for multi-component alloys according to the CALPHAD (CALculation of PHase Diagrams) - methodology
 - Database development for
 - * Bi-In-Sn-Zn system for lead-free soldering
 - * Ga-In-Si system for the growth of Si nanowires via the vapor-liquid-solid technique
 - Calculation of multi-component phase diagrams using commercial thermodynamic software and databases
- Equilibrium and non-equilibrium thermodynamics

Scientific projects and collaborations

Projects:

- Involved in European COST-actions on the development of multi-component alloys
 - COST 531: Lead-free solder materials (2003 - 2007, finished)
 - COST 535: Thermodynamics of alloyed aluminides (December 2003 - December 2007)
 - COST MP0602: Advanced solder materials for high-temperature application – their nature, design, process and control in a multiscale domain (May 2007 - May 2011)
 - * Representative for Belgium in the Management Committee
 - * Coordinator of Work Group 3 on 'Processes at the interface'
 - * Coordinator of a group project on 'Complex modelling of the microstructural changes occurring in the interdiffusion zone of Pb-free solder joints'.
- Approved project applications for national funding
 - OT/07/040: Quantitative phase-field modelling of coarsening processes in lead-free solder joints (October 2007 - September 2011). Financing for 1 Ph.D. - student for 4 years, 10 computing nodes for the HPC (High Performance Computer) of the K.U.Leuven.
 - IMEC PhD grant: Thermodynamic and kinetic study of nanoscopic systems: growth of nanowires. Financing for 1 Ph.D. - student for 4 years (November 2007 - October 2011).

Scientific manifestations:

- Organizer, together with L. Vanherpe, of a minisymposium on "Towards realistic 3-dimensional phase-field simulations for the evolution of polycrystalline structures", on the SIAM-conference on Mathematical aspects of materials science, May 2008, Philadelphia. Speakers: L.Q. Chen, L. Gránásy, M. Dorr, Y. Suwa, L. Vanherpe.
- Organizer, together with G. Samaey (postdoc at the Computer Science department, K.U.Leuven), of a 'Workshop on kinetic simulation techniques for material processes at the atomistic scale' in July 2008 in Leuven.

- Member of the scientific committee of "Second decennial symposium on phase-field modelling in materials science", Aachen, September 2009 (chairmen I. Steinbach and L.-Q. Chen).

International stays

- **February-March 2008:** School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138 USA.
- **September 2008 - August 2009:** Physics Department, Lawrence Livermore National Laboratories, California, USA.

Collaborations (ongoing scientific work):

- Francesca Iacopi (senior researcher at IMEC, Leuven), since September 2006: Thermodynamic and kinetic study and characterization of nanoscopic systems.
- Britta Nestler, Frank Wendler (Karlsruhe University of Applied Sciences), since September 2005: Comparison of the multiphase-field model (Karlsruhe) and the continuum phase-field model (Leuven), for microstructure evolution in multi-component alloys and grain growth.
- Sacha Kodentsov (Technische Universiteit Eindhoven), since December 2004: Diffusion couple experiments Al-Ni-Ti. COST-MP0602 on lead-free solders.
- Frans Spaepen (Harvard University), since January 2007: Simulation of grain growth in anisotropic systems. Effect of thermal noise on grain growth.
- Liesbeth Vanherpe, Giovanni Samaey, Stefan Vandewalle, Dirk Roose (Computer science department, K.U.Leuven) Development of efficient numerical techniques for the solution of phase-field equations. Multi-scale simulation techniques for microstructure evolution.
- Bert Rodiers (Senior software developer at LMS International, Haasrode), since September 2002: C++-implementation of the phase-field model
- Alexis Miroux, S. van der Zwaag, (Technische Universiteit Delft), since September 2007: Study of the jerky motion of grain boundaries during recrystallization in Al-alloys containing AlMn-precipitates.
- Patrice Turchi, Jim Belak, Milo Dorr, Ming Tang (LLNL), since September 2008: Large-scale phase field simulations.

Teaching and student guiding

Courses

- Exercises Thermodynamics, Bachelor in Applied Sciences, K.U.Leuven (Academic year: 2002-2003, 2003-2004, 2004-2005)

- Chemical Materials Science II: Thermodynamic modelling and the calculation of phase diagrams, Master of Science in Materials Engineering, K.U.Leuven (Academic year: 2006-2007, 2007-2008)

Supervision bachelor theses

- Jens Conderaerts, Eline De Roose, Saphia Rachidi, Studie van Ga-In-Si legeringen voor de groei van Si-nanodraden via de damp-vloeibaar-vast methode, Bachelor in Engineering with a major in Materials Science, K.U.Leuven, 2006-2007.

Supervision master theses

- Liesbeth Vanherpe, Numerical simulation of grain growth, Master in Computer Science, Faculty of Engineering, K.U.Leuven, 2003-2004.
- Jiang Zhu, In-situ observation of microstructure evolution in metals using a Confocal Scanning Laser Microscope, MME-program, Dept. Metallurgy and Materials Engineering, K.U.Leuven, 2003-2004.
- An Serbruyns, Experimental study of phase-equilibria in the Aluminum-Nickel-Titanium system by means of the diffusion couple technique, Master of science in Materials Engineering, Faculty of Engineering, K.U.Leuven, 2005-2006.
- Jeroen Heulens, Study of the solidification of $\text{SiO}_2\text{-Al}_2\text{O}_3\text{-CaO}$ -slags with the water-cooled probe technique, Master of science in Materials Engineering, Faculty of Engineering, K.U.Leuven, 2006-2007.
- WeiWei Chen, Determination of liquidus and solidus temperatures of the Ga-In-Si system for the growth of Si nanowires via the vapour-liquid-solid technique, MME-program, Dept. Metallurgy and Materials Engineering, K.U.Leuven, 2006-2007.
- Joris Roeck, Thermodynamic and kinetic study of the growth of semi-conductor GeSi-nanowires via the vapour-liquid-solid technique, Master of Science in Materials Engineering, Faculty of Engineering, K.U.Leuven, 2007-2008.

Supervision doctoral theses

- Liesbeth Vanherpe (Dept. Computer Science, K.U.Leuven), "Development, analysis and implementation of parallel multigrid algorithms for the numerical simulation of mathematical models for grain growth", started at October 1, 2005.
- An Serbruyns (Dept. Metallurgy and Materials Engineering, K.U.Leuven), "Quantitative phase-field simulations of the morphological evolutions in lead-free solder joints", started at October 1, 2006.
- Jeroen Heulens (Dept. Metallurgy and Materials Engineering, K.U.Leuven), "Phase-field modelling of the solidification of oxidic systems", started at October 1, 2007.
- Yann Eichhammer (Dept. Metallurgy and Materials Engineering, K.U.Leuven), "Thermodynamic and kinetic study of nanoscopic systems: growth of nanowires", started at November 1, 2007.

Further diplomas, education, interests

Attended courses (outside the regular curriculum of materials engineering)

In the last year of the masters and the first two years of the Ph.D., a number of courses were followed from the Master program for Physics and the Master program for Computer Science at the K.U.Leuven, namely

- Master in Physics, K.U.Leuven:
 - Statistical mechanics
 - Solid state physics
 - Mathematics for physical problems
 - Physics of fluids
- Master in Computer Science, K.U.Leuven
 - Numerical methods for the solution of partial differential equations
 - Algorithms for large-scale numerical simulations
 - Algorithms for parallel computing
 - Design and implementation of scientific software
- Doctoral courses, K.U.Leuven
 - Continuum modelling of material properties
 - Academic english

Attended workshops and seminars¹

- Workshop on phase-field models with stress/strain coupling, ACCESS, Aachen, April 9-10, 2003
- International seminar on heterogeneous multicomponent equilibria, 18th MSIT meeting, Stuttgart, Februari 29 - March 6, 2004
- Workshop on the diffusion couple technique (COST-535), Düsseldorf, December 5-7, 2004
- 19th MSIT-meeting, Stuttgart, Germany, February 2005.
- An introduction to atomistic modeling techniques, IMEC, Leuven, September 27-28 and October 3-4, 2005.
- Méthodes de Champs de Phase, Ecole de Physique, Les Houches, March 27-31, 2006
- Thermo-Calc workshop and training, ACCESS, Aachen, September 28-29, 2006.
- Polymorphism in Condensed Matter (POLCOM), Max Planck Institute for the Physics of Complex Systems, Dresden, November 13-17, 2006.

¹Without contribution. See list of oral and poster presentations for an overview of attended conferences with contribution

- GraSMech course on "Micromechanics of heterogeneous materials : modelling and computation", U.C.L, Louvain-la-Neuve, Belgium, February 14-16, 2007.
- 21st annual MSIT-meeting on "Multicomponent Heterogeneous Equilibria", Schloss Ringberg, Germany, February 26 - March 2, 2007.

Computer Skills

- Operating systems: basic knowledge of Windows and Linux/Unix
- Scientific software: Matlab, Maple, Ansys, Thermo-Calc & DICTRA, Pandat
- Application software: MS Word, MS Excel, MS Powerpoint, LaTeX, CorelDRAW
- Programming languages: Matlab, basic knowledge of Fortran, C/C++, Scheme and Labview

Languages

- Dutch: mother tongue
- English: very good knowledge
- French: basic knowledge

Other

- Driving licence (the Belgian driving licence B)
- Diploma of higher degree in ballet (part-time education)
- Diploma of higher degree in piano (part-time education)