

# Publication List Nele Moelans

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## Publications in international journals with S.C.I. impactfactor

1. N. Moelans, K.C. Hari Kumar, P. Wollants. Thermodynamic optimization of the lead-free solder system Bi-In-Sn-Zn. *J. Alloys Comp.*, 360(1-2), 98-106, 2003.
2. N. Moelans, B. Blanpain, P. Wollants. A phase field model for the simulation of grain growth in materials containing finely dispersed incoherent second-phase particles. *Acta Mater.* 53(6), 1771-1781, 2005.
3. N. Moelans, B. Blanpain, P. Wollants. Phase field simulations of grain growth in two-dimensional systems containing finely dispersed second-phase particles. *Acta Mater.*, 54(4), 1175-1184, 2006.
4. N. Moelans, B. Blanpain, P. Wollants. Pinning effect of second-phase particles on grain growth in thin films studied by 3D phase field simulations. *Acta Mater.*, 55, 2173-2182, 2007.
5. L. Vanherpe, N. Moelans, B. Blanpain, S. Vandewalle. Bounding box algorithm for three-dimensional phase field simulations of microstructural evolution in polycrystalline materials. *Phys. Rev. E*, 76(5), 056702, 2007.
6. F. Iacopi, P.M. Vereecken, M. Schaekers, M. Caymax, N. Moelans, B. Blanpain, O. Richard, C. Detavernier, H. Griffiths. Plasma-enhanced chemical vapor deposition growth of Si nanowires with low melting point metal catalyst: an effective alternative to Au-mediated growth. *Nanotechnology*, 18, 505307, 2007.
7. N. Moelans, B. Blanpain, P. Wollants. An introduction to phase-field modeling of microstructure evolution. *Calphad – Computer coupling of phase diagrams and thermochemistry*, 32, 268-294 (2008).
8. N. Moelans, B. Blanpain, P. Wollants, Quantitative phase-field approach for simulating grain growth in anisotropic systems with arbitrary inclination and misorientation dependence, *Phys. Rev. Lett.*, 101, n 025502, 2008.  
*Also selected for the July 15, 2008 issue of Virtual Journal of Biological Physics Research (<http://www.vjbio.org>).*

9. N. Moelans, B. Blanpain, P. Wollants, Quantitative analysis of grain boundary properties in a generalized phase field model for grain growth in anisotropic systems, *Phys. Rev. B*, 78 (2), n 024113 (2008).  
Also selected for the August 1, 2008 issue of *Virtual Journal of Biological Physics Research* (<http://www.vjbio.org>).
10. N. Moelans, A phase-field model for multi-component and multi-phase systems, *Arch. Metall. Mater.*, 53 (4), 1149-1156 (2008).  
Proceedings of TOFA (Thermodynamics of alloys) 2008.
11. Y. Eichhammer, J. Roeck, N. Moelans, F. Iacopi, B. Blanpain, M. Heyns, Calculation of the Au-Ge phase diagram for nanoparticles, *Arch. Metall. Mater.*, 53 (4), 1133-1139 (2008).  
Proceedings of TOFA (Thermodynamics of alloys) 2008.
12. N. Moelans, F. Wendler, B. Nestler, Comparative study of two phase-field models for multi-grain structures. *Comp. Mater. Sci.*, 46 (2), 479-490 (2009)
13. N. Moelans, F. Spaepen, P. Wollants. Grain growth in thin films with a fiber texture studied by phase-field simulations and mean field modeling. *Phil. Mag.*, 90, 501-523, 2010.
14. J. Heulens and N. Moelans. On the rotation invariance of multi-order parameter models for grain growth. *Scripta Mater.*, 62, 827-830, 2010.
15. L. Vanherpe, N. Moelans, B. Blanpain, S. Vandewalle. Pinning effect of spheroid second-phase particles on grain growth studied by three-dimensional phase field simulations. *Comp. Mater. Sci.*, 49, 340-350, 2010.
16. N. Moelans, G. Samaey. Editorial special issue on Multiscale Modeling of Moving Interfaces in Materials. *Mathematics and Computers in Simulation*, 80 (7), 1359-1360, 2010.
17. N. Moelans. A quantitative and thermodynamically consistent phase-field interpolation function for multi-phase systems. *Acta Mater*, 59, 1077-1086, 2011.
18. J. Heulens, B. Blanpain, N. Moelans. A phase-field model for isothermal crystallization for oxide melts. *Acta Mater*, 59, 2156-2165, 2011.
19. Y. Eichhammer, M. Heyns, N. Moelans. Calculation of phase equilibria for an alloy nanoparticle in contact with a solid nanowire. *CALPHAD – Computer Coupling of Phase Diagrams and Thermochemistry*, 35, 173-182, 2011.
20. L. Vanherpe, N. Moelans, B. Blanpain, S. Vandewalle. Bounding box framework for efficient phase field simulation of grain growth in anisotropic systems. *Comp. Mater. Sci.*, 50, 2221-2231, 2011.
21. J. Heulens, B. Blanpain, N. Moelans. Phase field analysis of a ternary two-phase diffusion couple with multiple analytical solutions. *Acta Mater*, 59, 3946-3954, 2011.
22. J. Heulens, B. Blanpain, N. Moelans. Analysis of the isothermal crystallization of CaSiO<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> melt through in-situ observations. *J. Ceram. Soc*, 31, 1873-1879, 2011.
23. J. Heulens, B. Blanpain, N. Moelans. Phase field modeling of the crystallization of FeOx-SiO<sub>2</sub> melts in contact with an oxygen-containing atmosphere. *Chemical Geology*, 290, 156-162, 2011.

24. N. Moelans, G. Samaey. Editorial special issue on Multiscale simulation of heterogeneous materials and coupling of thermodynamic models. *Comp. Mater. Sci.*, 66, 1-2, 2013.
25. A. Durga, P. Wollants, N. Moelans. Evaluation of interfacial excess contributions in different phase-field models for elastically inhomogeneous systems. *Modelling Simul. Mater. Sci. Eng.*, 21, 055018, 2013.
26. N. Moelans, A. Godfrey, Y.B. Zhang, D. Juul Jensen. Phase-field simulation study of the migration of recrystallization boundaries. *Phys. Rev. B*, 88, no 054103, 2013.
27. Minh O, George Vakanas, Nele Moelans, Masanori Kajihara, Wenqi Zhang. Formation of compounds and Kirkendall vacancy in the Cu-Sn system. *Microelectronic Engineering*, 120, 133-137, 2014.
28. Kunok Chang and Nele Moelans. Effect of grain boundary energy anisotropy on highly-textured grain structures studied by phase field simulations. *Acta Mater.*, 64, 443-454, 2014.
29. Jing-Jing Liu, Gong Chen, Peng-Cheng Yan, Bart Blanpain, Nele Moelans, Muxing Guo. In-Situ observation of isothermal CaSiO<sub>3</sub> crystallization in CaOAl<sub>2</sub>O<sub>3</sub>SiO<sub>2</sub> melts: a study of the effects of temperature and composition. *Journal of Crystal Growth*, 402, 1-8, 2014.
30. Hamed Ravash, Jef Vleugels, Nele Moelans. Three-dimensional phase-field simulation of microstructural evolution in three-phase materials with different diffusivities. *Journal of Materials Science*, 49, 7066-7072, 2014.
31. Yuanyuan Guan, Nele Moelans. Influence of the solubility range of intermetallic compounds on their growth behavior in hetero-junctions. *J. Alloys Comp.*, 635, 289-299, 2015.
32. Kunok Chang, Nele Moelans. Phase-field simulations of the interaction between a grain boundary and an evolving second-phase particle. *Phil. Mag. Letters*, 95 (4), 202-210, 2015.
33. A. Durga, P. Wollants, N. Moelans. A quantitative phase-field model for two-phase elastically inhomogeneous systems. *Comp. Mater. Sci.*, 99, 81-95, 2015.
34. I. Bellemans, N. Moelans, K. Verbeken. Phase field modelling of the attachment of metallic droplets to solid particles in liquid slags: influence of interfacial energies and slag supersaturation. *Comp. Mater. Sci.*, 108, 348-357, 2015.
35. Nabi Nabiollahi, Nele Moelans, Mario Gonzalez, Joke De Messemaeker, Christopher J. Wilson, Kristof Croes, Eric Beyne and Ingrid De Wolf. Microstructure Simulation of Grain Growth in Cu Through Silicon Via Using Phase-Field Modeling. *Microelectronics reliability*, 55, 765-770, 2015.
36. Evelien De Wilde, Inge Bellemans, Mieke Campoorts, Abdul Khaliq, Kim Vanmeensel, David Seveno, Muxing Guo, Akbar Rhamdhani, Geoff Brooks, Bart Blanpain, Nele Moelans, Kim Verbeken. Wetting behaviour of Cu based alloys on spinel substrates in pyrometallurgical context. *Materials Science and Technology*, 31, 1925-1933, 2015.
37. Inge Bellemans, Evelien De Wilde, Nele Moelans, Kim Verbeken. Phase field modelling of the attachment of metallic droplets to solid particles in liquid slags: Influence of particle characteristics. *Acta Mat.*, 101,172-180, 2015.

38. Yuan Yuan, Dajian Li and Nele Moelans. Comment on A numerical method to determine interdiffusion coefficients of  $\text{Cu}_6\text{Sn}_5$  and  $\text{Cu}_3\text{Sn}$  intermetallic compounds. *Intermetallics*, 36, 95-97, 2016.
39. Yuan Yuan, Yuanyuan Guan, Dajian Li, Nele Moelans. Investigation of diffusion behavior in Cu-Sn solid state diffusion couples. *Journal of Alloys and Compounds*, 661, 282-293, 2016.
40. E. De Wilde, I. Bellemans, M. Campforts, M. Guo, B. Blanpain, N. Moelans, K. Verbeken. Sessile drop evaluation of high temperature copper/spinel and slag/spinel interactions. *Transactions of Nonferrous Metals Society of China*, 26, 2770-2783, 2016.
41. A. Gil Santos, N. Moelans, N. Hort and O. Van der Biest. Identification and description of intermetallic compounds in Mg-Si-Sr cast and heat-treated alloys *Journal of Alloys and Compounds*, 669, 123-133, 2016.
42. E. De Wilde, I. Bellemans, M. Campforts, M. Guo, B. Blanpain, N. Moelans and K. Verbeken. Origin and sedimentation of Cu-droplets sticking to spinel solids in pyrometallurgical slags. *Materials Science and Technology*, 32 (18), 1743-2847, March 2016. (<http://dx.doi.org/10.1080/02670836.2016.1151998>).
43. Inge Bellemans, Evelien De Wilde, Nele Moelans en Kim Verbeken. Phase field simulation study of the attachment of metallic droplets to solid particles in liquid slags based on real slag-spinel micrographs. *Comp. Mater. Sci.*, 118, 269-278, 2016.
44. Jingjing Liu, Jeroen Heulens, Mu-Xing Guo, Nele Moelans. Isothermal Crystal Growth Behavior of  $\text{CaSiO}_3$  in Ternary Oxide Melts. *Journal of Inorganic Materials*, Vol 31, n 5, 547-554, 2016.
45. Jingjing Liu, Ji Zou, Muxing Guo, Nele Moelans. Phase field simulation study of the dissolution behavior of  $\text{Al}_2\text{O}_3$  into  $\text{CaO-Al}_2\text{O}_3\text{-SiO}_2$  slags. *Computational Materials Science*, 119, 9-18, 2016.
46. Yuan Yuan, Dajian Li, Yuanyuan Guan, Hans J. Seifert, Nele Moelans. Investigation of the diffusion behavior in Sn-xAg-yCu/Cu solid state diffusion couples. *Journal of Alloys and Compounds*, 686, 794-802, 2016.
47. Hou Yanhui, Zheng Wan, Wu Zhenhua, Li Guangqiang, Nele Moelans, Muxing Guo, Babar Shahzad Khan. Study of Mn absorption by complex oxide inclusions in Al-Ti-Mg killed steels. *Acta Materialia*, 118, 8-16, 2016.
48. Evelien De Wilde, Inge Bellemans, Mieke Campforts, Muxing Guo, Bart Blanpain, Nele Moelans Kim Verbeken. Investigation of high temperature slag/copper/spinel interactions. *Metallurgical and Materials Transactions B*, 47, 3421-3434, 2016.
49. Vishal Yadav, Liesbeth Vanherpe, Nele Moelans. Effect of volume fractions on microstructure evolution in isotropic volume-conserved two-phase alloys: A phase-field study. *Comp. Mater. Sci*, 125, 297-308, 2016.
50. A. Gil Santos, I. Marco, N. Moelans, N. Hort and O. Van der Biest. Microstructure and degradation performance of biodegradable Mg-Si-Sr implant alloys. *Materials Science & Engineering C*, 71, 25-34, 2017.

51. A. Gil Santos, G. Szakacs, N. Moelans, N. Hort and O. Van der Biest. Microstructure and mechanical characterization of cast Mg-Ca-Si alloys. *Journal of Alloys and Compounds*, 694, 767-776, 2017.
52. Kunok Chang, Long-Qing Chen, Carl E. Krill and Nele Moelans. Phase-field simulation of highly textured 3-D grain structures. *Comp. Mater. Sci.*, 127, 67-77, 2017.
53. Evelien De Wilde, Inge Bellemans, Mieke Campforts, Muxing Guo, Kim Vanmeensel, Bart Blanpain, Nele Moelans, Kim Verbeken. Study of the effect of spinel composition on metallic copper losses in slags. *Journal of Sustainable Metallurgy*, 3, 416-427, 2017.
54. Hamed Ravash, Liesbeth Vanherpe, Jef Vleugels, Nele Moelans. Three-dimensional phase-field study of grain coarsening and grain shape accommodation in the final stage of liquid-phase sintering *Journal of the European Ceramic Society*, 37, 2265-2275, 2017.
55. Hamed Ravash, Jef Vleugels, Nele Moelans. Three-dimensional phase-field simulation of microstructural evolution in three-phase materials with different interfacial energies and different diffusivities. *Journal of Materials Science*, 52, 13852-13867, 2017.
56. Inge Bellemans, Evelien De Wilde, Lisa Claeys, Tim De Seranno, Mieke Campforts, Bart Blanpain, Nele Moelans, Kim Verbeken. Investigation of reactive origin for attachment of Cu droplets to solid particles. *Metallurgical and Materials Transactions B*, 48, 2459-2468, 2017.
57. Inge Bellemans, Evelien De Wilde, Nele Moelans, Kim Verbeken. Metal losses in pyrometallurgical operations - a review. *Advances in Colloid and Interface Science*. In press.  
<https://doi.org/10.1016/j.cis.2017.08.001>.
58. Vishal Yadav, Nele Moelans. Investigation on the existence of a 'Hillert regime' in normal grain growth. *Scripta Mater*, 142, 148-152, 2018.
59. Inge Bellemans, Vincent Cnockaert, Evelien De Wilde, Nele Moelans, Kim Verbeken. Metal droplet entrainment by solid particles in slags: an experimental approach. *Journal of sustainable metallurgy*. Published online: DOI 10.1007/s40831-017-0145-1
60. Inge Bellemans, Nele Moelans, Kim Verbeken. Phase-field modelling in extractive metallurgy. *Critical Reviews in Solid State and Materials Sciences*. Accepted, October 2017.
61. Inge Bellemans, Nele Moelans, Kim Verbeken. Influence of rigid body motion on the attachment of metallic droplets to solid particles in liquid slags : a phase field study. *Minerals & Metallurgical Processing journal*. Accepted October 2017.
62. Vishal Yadav, Nele Moelans. Comparison of coarsening behaviour in non-conserved and volume-conserved isotropic two-phase grain structures. *Scripta Mat.*, 146, 142-145, 2018.
63. Jingjing Liu, Ji Zou, Muxing Guo, Nele Moelans. Phase-field simulation and analytical modelling of CaSiO<sub>3</sub> growth in CaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> melts. *Comp. Mater. Sci.* Accepted, Dec 11, 2017.

## Contributions to books and compendiums

1. N. Moelans, N. Lebrun, P. Pierrot. Critical assessment of Ag-Cd-Cu system. In *Landolt-Börnstein, Group IV (Physical Chemistry)* Volume 11: Ternary Alloys Systems, Subvolume B: Noble Metals Systems, 2006.
2. N. Lebrun, N. Moelans, P. Pierrot. Critical assessment of Ag-H-Pd system. In *Landolt-Börnstein, Group IV (Physical Chemistry)* Volume 11: Ternary Alloys Systems, Subvolume B: Noble Metals Systems, 2006.
3. K.C. Hari Kumar, J. Gröbner, A. Malfliet N. Moelans. Critical assessment of Boron-Tungsten-Zirconium system. In *Landolt-Börnstein, Numerical data and Functional Relationships in Science and Technology (New Series). Group IV: Physical Chemistry.* Vol. 11E2, Ternary Alloy Systems. Phase Diagrams, Crystallographic and Thermodynamic Data Refractory Metal Systems. G. Effenberg, S. Ilyenko (Eds.), Springer-Verlag, Berlin, Heidelberg, 223-229, 2010.
4. N. Moelans et al., GP4 - Modeling and experimental investigation of the microstructural changes in the interdiffusion zone of leadfree solder joints. In COST Action MP0602 - Handbook of High-Temperature Lead-Free Soldering system: Vol. 3 Group Project Reports, ed. A. Kroupa, ISBN 978-80-905363-3-3, 2012.

## Scientific editor

1. Guest editor for a special issue of *Mathematics and Computers in Simulation (Elsevier)* on Multi-Scale Modeling of Moving Interfaces in Materials, N. Moelans and G. Samaey, 80(7), 1359-1564, 2010.
2. Guest editor for a special issue of *Computational Material Science (Elsevier)* on Multiscale Simulation of Heterogeneous Materials and Coupling of Thermodynamic Models, Vol 66, January 2013.

## Publications in journals without S.C.I. impact factor – Conference proceedings

1. N. Moelans, B. Coletti, J. Plessers, M. Straetemans, B. Blanpain, P. Wollants. Measurement of the oxygen potential of non-ferrous slags with an ex-situ electrochemical device. In *Metallurgical and Materials Processing Principles and Technologies (Yazawa International Symposium, San Diego, CA, USA)* Volume 1: Materials Processing Fundamentals and New Technologies, 509-515, Ed. by H.Y. Sohn, K. Itagaki, C. Yamauchi, and F. Kongoli, March 2-6, 2003.
2. N. Moelans. Berekenen van fase diagrammen voor loodvrije soldeerlegeringen op basis van Bi-In-Sn-Zn. *ATB Metallurgie* 42(3), 10-19, 2002.
3. N. Moelans, B. Blanpain, P. Wollants. Phase field simulations of grain growth in systems containing second-phase particles. *TMS Letters*, 2(2), 59-60, 2005.
4. N. Moelans, B. Blanpain, P. Wollants. A phase field model for grain growth and thermal grooving in thin films with orientation dependent surface energy. *Diffusion and Defect Data Part B (Solid State Phenomena)*, 129, 89-94, 2007.

5. F. Iacopi, P.M. Vereecken, M. Schaekers, M. Caymax, N. Moelans, B. Blanpain, C. Detavernier, H. Griffiths. Alternative catalysts for Si technology-compatible growth of Si nanowires. In Proceedings of the *MRS Spring meeting 2007, S. Francisco – joint session symp. DD/EE*, Vol 1018E, 1017-EE01-10, 2007.
6. L. Vanherpe, N. Moelans, B. Blanpain, S. Vandewalle. Three-dimensional phase field simulations of grain growth in materials containing finely dispersed second-phase particles. *Proceedings in Applied Mathematics and Mechanics (PAMM)*, 7(1), 2020001-2020002, 2008. Special Issue: 6th International Congress on Industrial and Applied Mathematics (ICIAM07) and GAMM Annual Meeting, Zurich, July, 16-20, 2007.
7. F. Iacopi, Y. Eichhammer, C. Massy, P.M. Vereecken, N. Moelans, O. Richard, D. Smeets, B. Blanpain S. De Gendt, M. Heyns. Indium assisted growth of Si-nanowires: perspectives and controlled VLS growth for CMOS applications. Proceedings of the *2008 MRS-Spring meeting*, Vol 1080E, 1080-O05-01, 2008.
8. N. Moelans, A. Serbruyns, J. Heulens, B. Blanpain, P. Wollants, L. Vanherpe, S. Vandewalle, B. Rodiers. Quantitative phase-field simulations of coarsening and growth in complex systems. *Proceedings of Mater. Sci. Technol. (MS&T) 2008, Session: Discovery and Optimization of Materials through Computational Design*, October 5-9, Pittsburgh, Pennsylvania, p 494-505.
9. N. Moelans, A. Miroux, E. Anselmino, S. van der Zwaag, B. Blanpain, P. Wollants. Phase-field simulations of coarsening of Al<sub>6</sub>Mn precipitates located on grain boundaries in Al alloys. *Collected Proceedings: Synergies of computational and experimental materials science, Vol 2: Materials characterization, computation and modeling, 138th TMS Annual Meeting & Exhibition*, Febr 15-19, 2009, San Francisco, California, p 303-310.
10. Nele Moelans, Liesbeth Vanherpe, Jeroen Heulens, Bert Rodiers, Bart Blanpain, Patrick Wollants, S. Vandewalle. Quantitative phase-field modeling of microstructure evolution in multi-component and multi-phase alloys. *Supplemental proceedings: Volume2: Materials Characterization, Computation, Modeling and Energy, TMS (The Minerals, Metals & Materials Society), 2010. Hume-Rothery Symposium: Configurational Thermodynamics of Materials*, Febr 14-18, Seattle, Washington, p 399-410.
11. A. Durga, Patrick Wollants, Nele Moelans. Phase-field model for solid state transformation in a two-phase binary system with elastic inhomogeneity. *Proceedings of International Symposium for Research Scholars, Department of Metallurgical and Materials Engineering, IIT Madras*, December 20-22, 2010.
12. Dorte Juul Jensen, Yubin Zhang, Andy Godfrey, Nele Moelans. Advancement in characterization and modeling of boundary migration during recrystallization. *Proceedings of 1st World Congress on Integrated Computational Materials Engineering*, Edited by J. Allison, P. Collins, G. Spanos. TMS (The Minerals, Metals & Materials Society), 2011, p19-26.
13. J. Heulens, B. Blanpain, N. Moelans. Crystallization of CaO.SiO<sub>2</sub> in a CaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> Melt: Computer simulations and in-situ experiments. Proceedings of the Fray International Symposium, Nov 27-Dec 1, 2011, Cancun, Mexico.
14. E. De Wilde, I. Bellemans, S. Vervynck, M. Campforts, K. Vanmeensel, N. Moelans, K. Verbeken, Towards a methodology to study the interaction between Cu droplets and spinel particles

- in slags. Proceedings of EMC 2013, European Metallurgical Conference, Weimar, Germany, June 23-26, 2013, Vol 1, 161-174.
15. E. De Wilde, K. Verbeken, M. Campforts, S. Vervynckt, K. Vanmeensel, N. Moelans, G. Godier, Characterization methodology for copper-droplet losses in slags. Proceedings of Copper 2013, Copper International Conference, Santiago, Chile, December 1-4, 2013, Vol 3, 189-197.
  16. Evelien De Wilde, Mieke Campforts, Greetje Godier, Kim Vanmeensel, Muxing Guo, Bart Blanpain, Nele Moelans, Kim Verbeken. Study of mechanically entrained copper droplet losses in slags due to their interaction with spinel solids. High Temperature Processing Symposium, 3-4 february, Australia, Melbourne, 2014, p79-81.
  17. Hamed Ravash, Eckard Specht, Jef Vleugels, Nele Moelans. 3D phase-field simulation and characterization of microstructure evolution during Liquid Phase Sintering. Proceedings of CIMTEC 2014, June 8-19, 2014, Montecatini Terme, Italy. In Advances in Science and Technology, 87, pp 132-138.
  18. N. Nabiollahi, N. Moelans, M. Gonzalez, J. De Messemaeker, C.J. Wilson, K. Croes, E. Beyne, I. De Wolf. Microstructure simulation of grain growth in Cu Through Silicon Via using phase-field modeling. Proceedings of the 15th International Conference on Thermal, Mechanical and Multi-Physics Simulation and Experiments in Microelectronics and Microsystems (EuroSimE), Ghent, Belgium, 7-9 April 2014. (art nr. 10.1109/EuroSimE.2014.6813848) IEEE.
  19. A. Gil-Santos, G.Szakacs, N.Moelans, N.Hort, O.Van der Biest. Thermodynamic calculation and experimental studies of phase relations in the Mg-Ca-Si-Sr system for degradable biomaterials. Proceedings of 6th Symposium on Biodegradable Metals. August 2014.
  20. Inge Bellemans, Nele Moelans, Kim Verbeken. Modelling the mechanical entrainment of metal droplets by solid particles in liquid slags. European Metallurgical Conference Proceedings, Düsseldorf, June 14-17, 2015, Vol 2, p 941-957, ISBN 978-3-940276-62-9.
  21. E. De Wilde, I. Bellemans, M. Campforts, M. Guo, K. Vanmeensel, B. Blanpain, N. Moelans, K. Verbeken. Wetting behaviour of spinel with copper to understand metallic copper losses to slags. In European Metallurgical Conference, Proceedings (2015), Vol 1, 3-17, Düsseldorf, June 14-17, 2015.
  22. Andrea Gil Santos, Gabor Szakacs, Nele Moelans, Norbert Hort, Omer Van der Biest. Correlation between mechanical behaviour and microstructure in the Mg-Ca-Si-Sr system for degradable biomaterials based on thermodynamic calculations. Proceedings Magnesium Technology 2015. 2015 TMS Annual Meeting & Exhibition, March 15-19, 2015, Orlando, Florida, US.
  23. A. Gil-Santos, I. Marco, G. Szakacs, N. Moelans, N. Hort, O. Van der Biest. Effect of composition on microstructure and properties of Mg-Si-Sr alloys for resorbable material applications. Proceedings of 7th Symposium on Biodegradable Metals. August 2015. Carovigno, Italy.
  24. N. Moelans, Y.B. Zhang, A. Godfrey, D. Juul Jensen. A phase-field simulation study of irregular grain boundary migration during recrystallization. Proceedings of the 36th Risoe International Symposium on Materials Science: Effects of Deformation Induced Structural Variations on Annealing Mechanisms. September, 7-11, 2015. DTU, Risoe Campus, Denmark. *IOP Conf. Series: Materials Science and Engineering*, 89, n° 012037, 2015. (doi:10.1088/1757-899X/89/1/012037)



25. I. Bellemans, V. Cnockaert, E. De Wilde, N. Moelans, K. Verbeken, Metal droplet entrainment by solid particles in slags: a combined phase field model and experimental approach, in: Proc. 5th International Slag valorisation symposium 2017; 2017: pp 181-184.
26. Inge Bellemans, Evelien De Wilde, Nele Moelans, Kim Verbeken. Metal Droplet entrainment by solid particles in slags: a combined phase field model and experimental approach, EMC 2017, June 25-28, Leipzig, Germany.
27. Omer Van der Biest, Andrea Gil-Santos, Norbert Hort, Rainer Schmid-Fetzer, Nele Moelans. Study on Mg-Si-Sr Ternary Alloys for Biomedical Applications, 2018 TMS Annual Meeting & Exhibition, March 11-15, Phoenix, Arizona, US, published in proceedings Magnesium Technology 2018: Magnesium Alloy Development: An LMD Symposium in Honor of Karl Kainer. Publication date, March 11, 2018.

## Oral presentations<sup>1</sup>

### \*Invited

1. **N. Moelans**, Phase-field simulations of grain growth in materials containing second-phase particles. Research Training Group 'Analysis, Numerics, and Optimization of Multiphase Problems', RTG - Berlin, Berlin, June 7, 2006.
2. **N. Moelans**, Phase field modelling of microstructure evolution. MSIT Meeting, Schloss Ringberg, Germany, February 25 - March 2, 2007.
3. **L. Vanherpe**, N. Moelans, B. Blanpain, S. Vandewalle. Three-dimensional simulations of grain growth in polycrystalline materials with the phase field method. Seminar on High Performance Computing, K.U.Leuven, Auditorium Kasteel Arenberg, Leuven, Belgium, April 27, 2007.
4. **N. Moelans**, L. Vanherpe, B. Blanpain, P. Wollants. Phase field simulations of grain growth in the presence of second-phase particles that evolve in time. Workshop on Phase-field models for the evolution of complex structures, Institut Henri Poincaré, Paris, June 4-6, 2007.
5. **N. Moelans** Phase field simulations for grain growth in materials containing second-phase particles, Materials Science Seminars at Harvard, Harvard University, Boston, February 28, 2008.
6. **N. Moelans**, L. Vanherpe, A. Serbruyns, B. Rodiers, Quantitative phase-field modeling of coarsening and grain growth in multi-component polycrystalline alloys, Materials Science and Technology Conference and Exhibition, MS & T'08 , October 5-9, 2008, David Lawrence Convention Center, Pittsburgh, Pennsylvania, USA. Symposium: "Discovery and Optimization of Materials through Computational Design"
7. **N. Moelans**, Quantitative phase-field modeling of grain growth and coarsening in multi-component alloys, Materials modelling seminar series, University of British Columbia, Vancouver, January 14, 2009.
8. **N. Moelans**, The phase-field method for mesoscale modeling of microstructure evolution, MSE Colloquium Series, Department of Materials Science and Engineering, University of California, Berkeley, March 5, 2009.

<sup>1</sup>The presenter is indicated in bold

9. **N. Moelans**, M. Tang, M.R. Dorr, J.-L. Fattebert, M.E. Wickett, J.F. Belak, P.E.A. Turchi. Representation of the phase-transition kinetics of binary alloys within a mesoscale phase-field model. Condensed Matter & Materials Science Seminar Series, Lawrence Livermore National Laboratory (LLNL), California, USA, August 20, 2009.
10. **N. Moelans**, A. Miroux, E. Anselmino, S. Van Der Zwaag. Phase field simulations of recrystallization in Al-Mn alloys containing Al<sub>6</sub>Mn precipitates. Euromat 2009, September, 7-10, 2009, Glasgow, UK. Symposium: Solid State Transformations  
*Highlight presentation (not invited)*
11. **N. Moelans**, A. Miroux, E. Anselmino, S. van der Zwaag. Phase field simulations of the coarsening of Al<sub>6</sub>Mn-precipitates located on a moving recrystallization front. Materials Science and Technology Conference and Exhibition, MS & T'09, October, 25-29, 2009, David Lawrence Convention Center, Pittsburgh, Pennsylvania, USA. Symposium: Integrated Computational and Experimental Investigations on Microstructure Evolution of Coarsening Systems.
12. **N. Moelans**, L. Vanherpe, J. Heulens, B. Rodiers. Quantitative Phase-Field Modeling of Microstructure Evolution in Multi-Component and Multi-Phase Alloys. TMS 2010 Annual Meeting & Exhibition, February 14-18, 2010, Washington State Convention Center, Seattle, WA. Hume-Rothery Symposium: Configurational Thermodynamics of Materials (In honor of the 2010 Hume-Rothery award recipient Didier de Fontaine)
13. **N. Moelans**, L. Vanherpe, J. Heulens, B. Rodiers. New directions in phase-field modelling of microstructure evolution in polycrystalline and multi-component materials. Third annual workshop of hero-m (KTH, Stockholm), Saltsjöbaden, Sweden, May 17-18, 2010.
14. **N. Moelans**, L. Vanherpe, J. Heulens, B. Rodiers. Phase-field modeling of microstructure evolution in multi-component alloys, COST MP0602 Industrial Seminar on Thermodynamics, Bratislava, April 6, 2010.
15. **J. Heulens**, B. Blanpain, N. Moelans. Phase field modeling of isothermal slag crystallization using FACT Databases. GTT-Technologies 12th Annual Workshop, June 16-18, 2010, Aachen, Germany.
16. **N. Moelans**. New directions in phase-field modeling of microstructure evolution in polycrystalline and multi-component alloys, Wuhan University of Science and Technology, Wuhan, China, September 13, 2010.
17. **N. Moelans**. 1) An introduction to phase-field modeling of microstructure evolution. 2) New directions in phase-field modeling for multi-component and multi-phase systems. School on Computational Modelling of Materials, Antwerp, Belgium, December 2-3, 2010.
18. **N. Moelans**. Quantitative phase-field modeling of growth and coarsening in multi-component alloys. Riso National Laboratory, Roskilde, Denmark, January 26 2011.
19. **D. Juul Jensen**, Y. Zhang, A. Godfrey, N. Moelans. Advancements in characterization and modelling of boundary migration during recrystallization. ICME2011–1st World Congress on Integrated Computational Materials Engineering, Seven Springs Mountain Resort, Seven Springs, PA, July 10-14, 2011.

20. **N. Moelans**, A. Godfrey, Yubin Zhang, D. Juul Jensen. Phase-field simulations of the formation of protrusions/retrusions on recrystallization boundaries. Work workshop, DTU, Risoe National Laboratory for sustainable energy, Roskilde, Denmark, Aug. 27-31, 2012.
21. **N. Moelans**. Quantitative phase-field modeling of growth and coarsening in polycrystalline materials. Workshop on Mesoscale and continuum scale modeling of materials defects, IPAM, Institute for Pure and Applied Mathematics, UCLA, California, USA, 13-16 November 2012.
22. **N. Moelans**, A. Godfrey, Yubin Zhang, D. Juul Jensen. A phase-field simulation study of irregular grain boundary migration during recrystallization. Final meeting of the scientific priority program (SPP1296) "Heterogenous nucleation and microstructure formation - Steps towards a system and scale-bridging understanding", Mercure Hotel Wings Frankfurt Airport, Germany, July 15-19, 2013.
23. **N. Moelans**. Phenomenological models for the thermodynamics and kinetics in nano-systems. WOG – School on atomistic simulation techniques, University of Antwerp, Belgium, 23-24 September 2013.
24. **N. Moelans**. Phase-field modeling of microstructure evolution in multi-component and polycrystalline materials. Imec-academy cursus on Materials and Interface modeling, Imec, Leuven, Belgium, 17-18 November 2014.
25. **N. Moelans**. Inaugural Lecture: Computational Thermodynamics – a powerfull approach to study microstructure evolution in materials. KU Leuven, Leuven, Belgium, 16 Febr. 2015.
26. **N. Moelans**. Inaugural Lecture: Unraveling interdiffusion effects at material interfaces – Learning from tensors and large-scale computer simulations. KU Leuven, Belgium, 9 March, 2017.
27. **Nele Moelans**, Hamed Ravash, Vishal Yadav. Phase-field modelling of microstructure evolution in two- and three-phase materials. Thermec 2018: International Conference on Processing & Manufacturing of advanced materials, Processing, Fabrication, Properties, Applications, July 8-13, 2018, Paris, France.

**\*Contributed**

1. **N. Moelans**, B. Blanpain, P. Wollants. Phase field simulations for grain growth in materials containing second-phase particles. TMS Annual meeting & exhibition, San-Francisco, California, February 14-17, 2005.
2. **N. Moelans**, B. Blanpain, P. Wollants. Phase field simulations of grain growth in materials containing second-phase particles. CALPHAD XXXIV, Maastricht, The Netherlands, May 22-27, 2005.
3. **N. Moelans**, B. Blanpain, P. Wollants. The effect of second-phase particles on grain growth in thin films studied by phase field simulations. EUROMAT, Prague, Czech Republic, September 5-8, 2005.
4. **N. Moelans**, B. Blanpain, P. Wollants. Phase field simulations for grain growth and thermal grooving in thin films. E-MRS 2006, Warsaw, Poland, September, 4-8 2006.

5. **N. Moelans**, L. Vanherpe, B. Blanpain, P. Wollants. Phase field simulations of the pinning effect of second-phase particles: Effect of particle shape, stability and interfacial properties. CALPHAD XXXVI, State College, Pennsylvania State, USA, May 6-11, 2007.
6. **L. Vanherpe**, N. Moelans, B. Blanpain, P. Wollants. Numerical simulations of 3D grain growth in materials containing finely dispersed second-phase particles. ICIAM07, Zurich, Switzerland, July 16-20, 2007.
7. **N. Moelans**, L. Vanherpe, B. Blanpain, P. Wollants. Phase field simulations of the pinning effect of second-phase particles on grain boundaries: Effect of particle shape and interfacial properties. EUROMAT, Nürenberg, Germany, September 10-13, 2007.
8. **A. Serbruyns**, L. Pandelaers, N. Moelans, B. Blanpain, P. Wollants, F. Iacopi, P.M. Vereecken. Determination of the Ga-In-Si phase diagram for the growth of Si nanowires via a vapour-liquid-solid technique. Thermo-Calc user meeting, Access, Aachen, Germany, September 27-28, 2007.
9. **J. Heulens**, M. Campforts, N. Moelans, B. Blanpain, P. Wollants. Microstructure formation during slag solidification. Thermo-Calc user meeting, Access, Aachen, Germany, September 27-28, 2007.
10. **An Serbruyns**, Nele Moelans, Ingrid De Wolf, Bart Blanpain, Patrick Wollants. Modelling interfacial reactions with Phase Field Method. Joint working group meeting, COST MP0602, Genoa, Italy, February 21-22, 2008.
11. **Nele Moelans**, Frans Spaepen, Bart Blanpain, Patrick Wollants. Quantitative phase field simulations of anisotropic grain growth in columnar thin films with a fiber texture. TMS annual meeting, New Orleans, March 9-13, 2008.
12. **An Serbruyns**, Nele Moelans, Ingrid De Wolf, Bart Blanpain, Patrick Wollants. Modelling Sn-Cu interfacial reactions with Phase Field Method. TMS annual meeting, New Orleans, March 9-13, 2008.
13. **L. Vanherpe**, N. Moelans, B. Blanpain, S. Vandewalle. Three-dimensional phase field simulations of grain growth in anisotropic systems. SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, May 11-14, 2008.
14. **N. Moelans**, L. Vanherpe, A. Serbruyns, B. Blanpain, P. Wollants, Phase field modelling of coarsening and grain growth, TOFA2008, Krakow, June 22-27 2008.
15. **Y. Eichhammer**, F. Iacopi, N. Moelans, B. Blanpain, P. Wollants, Calculation of phase diagrams for nanoparticles, TOFA2008, Krakow, June 22-27 2008.
16. **N. Moelans**, A. Miroux, E. Anselmino, S. van der Zwaag, B. Blanpain, P. Wollants. Phase field simulations of recrystallization in Al alloys containing Al<sub>6</sub>Mn precipitates. 2009 TMS Annual Meeting & Exhibition, Febr 15-19, 2009, San Francisco, California.
17. **J. Heulens**, N. Moelans, F. Verhaeghe, B. Blanpain, P. Wollants. Phase field modelling of slag solidification. 2009 TMS Annual Meeting & Exhibition, Febr 15-19, 2009, San Francisco, California.

18. **N. Moelans**. Effect of defects on microstructure evolution in the interdiffusion zone in Cu-Sn solder joints: A phase-field study. Mid-term meeting COST MP0602 ("Advanced Solder Materials for High Temperature Application - HISOLD"), April 15-17, 2009, Bochum, Germany.
19. **L. Vanherpe**, N. Moelans, B. Blanpain, S. Vandewalle. The effect of ellipsoid second-phase particles on grain growth studied by three-dimensional phase field simulations. 2nd Symposium on Phase-Field Modelling in Materials Science – PF09, August 30-September 2, 2009, Rolduc Abbey, Aachen, Germany.
20. **N. Moelans**, F. Spaepen. Quantitative phase field simulations of anisotropic grain growth in columnar thin films with a fiber texture. Euromat 2009, September, 7-10, 2009, Glasgow, UK. Symposium: Modelling of materials properties at mesoscale.
21. **Y. Eichhammer**, N. Moelans, B. Blanpain, F. Iacopi, M. Heyns. Calculation of thermodynamic equilibrium conditions between a liquid nanoparticle and a solid nanowire. Euromat 2009, September, 7-10, 2009, Glasgow, UK. Symposium: Synthesis and applications of nanowires.
22. **A. Durga**, K.C. Hari Kumar, N. Moelans, P. Wollants. Thermodynamic optimization of the Co-Zr system. APDIC International Conference, Third World Round Robin Seminar "Phase diagrams for energy saving", March 21-23, 2010, Montpellier 2 University, France.
23. **N. Moelans**. Phase field simulations of diffusion and growth in lead-free solder joints. Working group 3 meeting, COST MP0602("Advanced Solder Materials for High Temperature Application - HISOLD"), K.U.Leuven, Belgium, January 6-7, 2010.
24. **N. Moelans**. Phase field simulations of growth and coarsening in the interdiffusion zone of leadfree solder joints. CALPHAD XXXIX, Jeju, Korea, May 23-28, 2010.
25. **J. Heulens**, N. Moelans, B. Blanpain, P. Wollants. Phase field modeling of isothermal crystallization of metallurgical slags using FACT thermodynamic databases for oxide systems. CALPHAD XXXIX, Jeju, Korea, May 23-28, 2010.
26. **N. Moelans**. Use of the COST 531 database and diffusion mobility data in phase-field simulations. COST MP0602 (Advanced Solder Materials for High Temperature Application - HISOLD) annual joint working group meeting, April 7-9, 2010, Bratislava, April 7-9, 2010.
27. **A. Durga**, Patrick Wollants, Nele Moelans. Phase-field model for solid state transformation in a two-phase binary system with elastic inhomogeneity. International Symposium for Research Scholars (ISRS), Department of Metallurgical and Materials Engineering, IIT Madras, December 20-22, 2010.
28. **A. Durga**, Patrick Wollants, Nele Moelans. Phase-field model for solid state transformation in a two-phase system with elastic inhomogeneity in 2-D. Workshop on Multiscale Simulation of Heterogeneous Materials and Coupling of Thermodynamic Models, K. U. Leuven, Belgium, 12-14 January 2011.
29. **Jeroen Heulens**, B. Blanpain, N. Moelans. Phase field modeling of isothermal slag crystallization using FACT databases. Workshop on Multiscale Simulation of Heterogeneous Materials and Coupling of Thermodynamic Models, K. U. Leuven, Belgium, 12-14 January 2011.

30. **N. Moelans**. Phase field simulations of growth and coarsening in the interdiffusion zone of leadfree Ag-Cu-Sn/Cu joints. 2011 TMS Annual Meeting & Exhibition, Febr 27- March 3, 2011, San Diego, California.
31. **N. Moelans**, B. Sundman, A. Dinsdale, S. Fries. Combining phase-field and CALPHAD for systems containing intermediate phases with low solubility. 2011 TMS Annual Meeting & Exhibition, Febr 27- March 3, 2011, San Diego, California.
32. **N. Moelans**, A. Durga, Y. Guan, B. Sundman, A. Dinsdale, S. Fries. Modeling IMC growth in leadfree solder joints using the phase-field method coupled with the COST-531 thermodynamic database. Final COST MP0602 meeting, June 22-24, 2011, BRNO.
33. **Y. Guan**, Durga, A., N. Moelans. Simulation of microstructural changes in composite Sn-Ag-Cu solder alloys with Cu nanoparticles. Thermo-Calc user meeting, September 8-9, 2011, ACCESS, Aachen, Germany.
34. **N. Moelans**. Phase field simulations of growth and coarsening in the interdiffusion zone of lead-free solder joints. Euromat 2011, 12-15 September 2011, Montpellier, France. Symposium: D34 - Thermodynamics and phase equilibria; Modeling of phase diagrams.
35. **A. Durga**, P. Wollants, N. Moelans, Phase-field study of elastic effects on the growth of intermetallic precipitates in Cu-Sn lead-free solder system. Euromat 2011, 12-15 September 2011, Montpellier, France. Symposium: D34 - Thermodynamics and phase equilibria; Modeling of phase diagrams.
36. **J. Heulens**, B. Blanpain, N. Moelans. Crystallization of CaO.SiO<sub>2</sub> in a CaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> melt: computer simulation and in-situ experiments. Fray International Symposium, Nov 27-Dec 1, 2011, Cancun, Mexico.
37. **V. Yadav**, N. Moelans. Application of phase field crystal modeling to studying coupled grain boundary migration and grain rotation. MS&T 2011, Greater Columbus Convention Center, Columbus, Ohio, October, 16-20, 2011.
38. **A. Durga**, P. Wollants, N. Moelans. Elastic effects on aging in Cu/Sn-Ag-Cu lead-free solder joints: A phase-field study. TMS 2012, March 11-15, 2012, Orlando, Florida. Symposium: Computational Thermodynamics and Kinetics.
39. **V. Yadav**, N. Moelans. 3D Phase field simulation of phase coarsening in binary two phase system. TMS 2012, March 11-15, 2012, Orlando, Florida. Symposium: Computational Thermodynamics and Kinetics.
40. **A. Durga**, P. Wollants, N. Moelans. Phase-field modelling coupled with micro-elasticity applied to ageing in Sn-Cu/Cu and Sn-Ag-Cu/Cu lead-free solder joints. ESMC 2012, 8th European Solid Mechanics Conference, Graz, Austria, 9-13 July, 2012.
41. **E. De Wilde**, S. Vervynckt, M. Campforts, N. Moelans, K. Verbeken. Characterization Methodology for Cu-Droplet losses in Slags. EMC – European Metallurgical Conference, Weimar, Germany, June 23-26, 2013.
42. **A. Durga**, P. Wollants, N. Moelans. Phase-field Study of Phase Equilibria in Strained Cu-Sn System. CALPHAD XLII, San Sebastian, Spain, May 26-31, 2013.

43. **E. De Wilde**, K. Verbeken, M. Campforts, S. Vervynckt, K. Vanmeensel, N. Moelans, G. Godier. Characterization methodology for copper-droplet losses in slags. Copper International Conference, Santiago, Chile, December 1-4, 2013.
44. **Yuanyuan Guan**, Nele Moelans. Phase Field Study of the Growth of Intermetallic Compounds in MultiComponent Joints. MSE 2014, Materials Science and Engineering. September 23-25, 2014, Darmstadt, Germany.
45. **Hamed Ravash**, Eckard Specht, Jef Vleugels, Nele Moelans. Three-dimensional phase-field simulation and characterization of liquid-phase sintering. CIMTEC 2014, Montecatini Terme, Italy, June 8-19, 2014.
46. **Andrea Gil Santos**, Nele Moelans, Norbert Hort, Omer Van der Biest. Correlation between the mechanical behaviour with the microstructure in the Mg-Ca-Si-Sr system for degradable biomaterials based on thermodynamic calculations. 2015 TMS Annual Meeting & Exhibition, Symposium: Magnesium Technology, Florida 2015.
47. **A. Gil-Santos**, I. Marco, G. Szakcs, N.Moelans, N.Hort, O.Van der Biest. Effect of composition on microstructure and properties of Mg-Si-Sr alloys for resorbable material applications. 7th Symposium on Biodegradable Metals in Carovigno, Italy. August, 2015. (Poster and Oral Communication)
48. **A. Gil-Santos**, N.Moelans, N.Hort, O.Van der Biest. Experimental investigation for the thermodynamic modeling of the Mg rich corner in the Mg-Si-Sr system. Calphad XLIV Loano, Italy. May 31- June 5, 2015.
49. **Evelien De Wilde**, Inge Bellemans, Mieke Campforts, Muxing Guo, Kim Vanmeensel, Bart Blanpain, Nele Moelans, Kim Verbeken. Study of the wetting behaviour of spinel with copper and slag to understand metallic copper losses to slags. EMC2015 (European Metallurgical Conference), Düsseldorf, Germany, June 14-17, 2015.
50. **Inge Bellemans**, Nele Moelans, Kim Verbeken. Modelling the mechanical entrainment of metal droplets by solid particles in liquid slags. EMC2015 (European Metallurgical Conference), Düsseldorf, Germany, June 14-17, 2015.
51. **J. Liu**, J. Heulens, M. Guo, N. Moelans. Isothermal CaSiO<sub>3</sub> crystallization in CaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> melt: a combination of phase field simulations with in-situ experiments. CALPHAD XLIV, Loano, Italy, May 31- June 5, 2015.
52. **Hamed Ravash**, Jef Vleugels, Nele Moelans. 3D phase-field simulation and characterization of microstructure evolution during Liquid Phase Sintering. International Conference on Sintering 2014, August 24-28, 2014, Dresden, Germany.
53. **Nele Moelans**, Andy Godfrey, Yubin Zhang, Dorte Juul Jensen. A Phase-Field Simulation Study of Irregular Grain Boundary Migration during Recrystallization. 36th Risoe International Symposium on Materials Science: Effects of Deformation Induced Structural Variations on Annealing Mechanisms. September, 7-11, 2015. DTU, Risoe Campus, Denmark.
54. **Y. Yuan**, D. Li, N. Moelans. Determination of diffusion parameters of the intermetallic compounds in Sn/ Cu and Sn-xAg-yCu/Cu diffusion joints. CALPHAD XLV, May 29-June 3, Awaji Yumebutai International Conference Center, Awaji Island, Hyogo, Japan, 2016.

55. **Inge Bellemans**, Evelien De Wilde, Nele Moelans, Kim Verbeken. Wettability of metal droplets on solid particles in liquid slags. Micromast, Brussels, 5-8 September 2016.
56. **Inge Bellemans**, Nele Moelans, Kim Verbeken. Metal Droplet entrainment by solid particles in slags: a combined phase field – experimental approach. 8th International Conference on Multiscale Materials Modeling MMM2016, 9-14 October, 2016, Dijon, France.
57. **Inge Bellemans**, Evelien De Wilde, Nele Moelans, Kim Verbeken. Metal Droplet entrainment by solid particles in slags: a combined phase field model and experimental approach, EMC 2017, June 25-28, Leipzig, Germany.
58. **Omer Van der Biest**, Andrea Gil-Santos, Norbert Hort, Rainer Schmid-Fetzer, Nele Moelans. Study on Mg-Si-Sr Ternary Alloys for Biomedical Applications. TMS 2018, 147th Annual Meeting & Exhibition, March 11-15, Phoenix, Arizona, US. Symposium: Magnesium Alloy Development: An LMD Symposium in Honor of Karl Kainer.
59. **Hong Liu**, F.X. Lin, P. Zhao, Y. Wang, J.F. Nie, N. Moelans. Nucleation and transmission of co-zone {101-2} deformation twins in Mg: A phase field simulation study. EMMC16 (European Mechanics Society), Nantes, France, March 26-28, 2018. In session S21 Advanced modelling techniques: phase field and diffuse-interface approaches.

## Poster presentations<sup>1</sup>

### \*Awarded

1. **N. Moelans**, B. Blanpain, P. Wollants. 3D Phase field simulations of grain growth in thin films: pinning effect of second-phase particles and thermal grooving, Gordon Research Conference on High Temperature Materials, Processes and diagnostics, Colby College, Waterville, ME, July 16-21 2006.  
*Ph. D. poster award: honorable mentioning for frontier research*
2. **A. Durga**, P. Wollants, N. Moelans. New Quantitative Phase-Field Model for Elastically Inhomogeneous Systems. CALPHAD XLII, San Sebastian, Spain, May 26-31, 2013. *CALPHAD post award. Best poster presented at CALPHAD XLII Conference, San Sebastian, Spain, 2013.*

### \*Full list

1. **N. Moelans**, K.C. Hari Kumar, P. Wollants. Bi-In-Sn-Zn system for lead-free soldering. CALPHAD XXXII, La Malbaie, Quebec, Canada, May 25-30, 2003.
2. **N. Moelans**, B. Blanpain, P. Wollants. Phase field simulations for grain growth in the presence of second-phase particles. TOFA, Vienna, Austria, September 12-17, 2004.
3. **J. Lacaze**, P. Wollants, N. Moelans, K.C. Hari Kumar, G. Cacciamani, R. Ferro. Critical assessment of the Fe-Ni-Ti system. TOFA, September 12-17, 2004, Vienna Austria, 2004.
4. **N. Moelans**, B. Blanpain, P. Wollants. 3D Phase field simulations of grain growth in thin films: pinning effect of second-phase particles and thermal grooving”, Gordon Research Conference

<sup>1</sup>The presenter is indicated in bold



on High Temperature Materials, Processes and diagnostics, Colby College, Waterville, ME, July 16-21 2006.

*Ph. D. poster award: honorable mentioning for frontier research*

5. **N. Moelans**, F. Wendler, B. Nestler. A comparison between continuum field and multi-phase field models for grain growth. CALPHAD XXXVI, State College, Pennsylvania State, USA, May 6-11, 2007.
6. A. Serbruyns, L. Pandelaers, **N. Moelans**, B. Blanpain, P. Wollants, F. Iacopi, P.M. Vereecken. Determination of the Ga-In-Si phase diagram for the growth of Si nanowires via a vapour-liquid-solid technique. CALPHAD XXXVI, State College, Pennsylvania State, USA, May 6-11, 2007.
7. **A. Serbruyns**, A. Kodentsov, J. De Keyzer, N. Moelans, B. Blanpain, P. Wollants. Phase Equilibria in the Aluminium-Nickel-Titanium System. CALPHAD XXXVI, State College, Pennsylvania State, USA, May 6-11, 2007.
8. **N. Moelans**, F. Wendler, B. Nestler. A comparison between continuum field and multi-phase field models for grain growth. Workshop on Phase-field models for the evolution of complex structures, Institut Henri Poincaré, Paris, June 4-6, 2007.
9. **L. Vanherpe**, N. Moelans, B. Blanpain, S. Vandewalle. Bounding box algorithm for three-dimensional phase field simulations of grain growth. Workshop on Phase-field models for the evolution of complex structures, Institut Henri Poincaré, Paris, June 4-6, 2007.
10. **Nele Moelans**, Frans Spaepen. Grain growth simulations with Langevin noise. TMS annual meeting, New Orleans, March 9-13, 2008.
11. **A. Serbruyns**, N. Moelans, B. Blanpain, P. Wollants, Phase field modelling of interfacial reactions in lead-free solder systems, TOFA2008, Krakow, June 22-27 2008.
12. **Nele Moelans**, Frans Spaepen. Grain growth simulations with Langevin noise. Workshop on multi-scale modeling of moving interfaces in materials, Leuven, July 2-4, 2008.
13. **Nele Moelans**, Bart Blanpain, Patrick Wollants. Quantitative phase-field approach for simulating grain growth in anisotropic systems with arbitrary inclination and misorientation dependence, Workshop on multi-scale modeling of moving interfaces in materials, Leuven, July 2-4, 2008.
14. **N. Moelans**, 3D phase field simulations of grain growth in thin films: pinning effect of second-phase particles and thermal grooving, Materials Science and Technology Conference and Exhibition, MS& T'08, David Lawrence Convention Center, Pittsburgh, Pennsylvania, USA, Symposium "Discovery and Optimization of Materials through Computational Design", October 5-9, 2008.
15. **A. Serbruyns**, N. Moelans, B. Blanpain, P. Wollants. A phase field model for the study of microstructure evolution in lead-free solder joints. 2009 TMS Annual Meeting & Exhibition, Febr 15-19, 2009, San Francisco, California.
16. **J. Heulens**, N. Moelans, F. Verhaeghe, B. Blanpain, P. Wollants. Isothermal multiphase field model for slag solidification. 2nd Symposium on Phase-Field Modelling in Materials Science – PF09, August 30-September 2, 2009, Rolduc Abbey, Aachen, Germany.

17. **A. Durga**, N. Moelans, P. Wollants. Phase-field simulation of spinodal decomposition in the Ag-Pd system. COST MP0602 (Advanced Solder Materials for High Temperature Application - HISOLD) annual joint working group meeting, April 7-9, 2010, Bratislava, April 7-9, 2010.
18. **J. Heulens**, N. Moelans, B. Blanpain, Phase-field analysis of a ternary two-phase diffusion couple with multiple analytical solutions. Workshop on Multiscale Simulation of Heterogeneous Materials and Coupling of Thermodynamic Models, K. U. Leuven, Belgium, 12-14 January 2011.
19. **H. Ravash**, N. Moelans, 3-dimensional phase-field model for liquid phase sintering of CIGS, Gordon Research Conference Physical Metallurgy "Evolution of Metals Structures: Modeling, Characterization and Design", Stonehill College, Easton MA, July 31- Aug 5, 2011. (also presented on the Kenyan conference)
20. **N. Moelans**, Microstructure simulation models for the growth of intermediate phases with low solubility, Gordon Research Conference Physical Metallurgy "Evolution of Metals Structures: Modeling, Characterization and Design", Stonehill College, Easton MA, July 31- Aug 5, 2011.
21. **N. Moelans**, A. Godfrey, Y.B. Zhang, D. Juul Jensen, Phase-field simulations of the formation of protrusions/retrusions on recrystallization boundaries, Euromat 2011, Montpellier, France, Sept 12-15, 2011. Symposium C12-Solid state transformations.
22. **V. Yadav**, N. Moelans. Phase field crystal simulation of curvature driven grain boundary migration. TMS 2012, March 11-15, 2012, Orlando, Florida. Symposium: Solid-state Interfaces II: Toward an atomistic-scale understanding of structure, properties and behavior through theory and experiment.
23. **A. Durga**, P. Wollants, N. Moelans. New Quantitative Phase-Field Model for Elastically Inhomogeneous Systems. CALPHAD XLII, San Sebastian, Spain, May 26-31, 2013. *CALPHAD post award. Best poster presented at CALPHAD XLII Conference, San Sebastian, Spain, 2013.*
24. **Yuan Yuan**, Yuanyuan Guan, Nele Moelans. Validation of different models for simulating the diffusion controlled growth of intermetallic compounds. CALPHAD XLII, San Sebastian, Spain, May 26-31, 2013.
25. **Y. Guan**, N. Moelans. Investigation of solubility range on the growth kinetics of intermetallic phases in hetero-junctions. CALPHAD XLIII, Central South University, Changsha, June 1-6, 2014.
26. **Yuanyuan Guan**, Nele Moelans. Influence of the solubility range of intermetallic compounds on their growth behaviour in hetero-junctions. Junior Euromat 2014, Lausanne, Switzerland, July 21-25.
27. **Inge Bellemans**, Nele Moelans, Kim Verbeken. The influence of interfacial energy and particle characteristics on the attachment of metallic droplets to solid particles in liquid slags. Third International Symposium on Phase Field Method – PFM 2014, State College, Pennsylvania, August 26-29, 2014.
28. **A. Gil-Santos**, G.Szakacs, N.Moelans, N.Hort, O.Van der Biest. Thermodynamic calculation and experimental studies of phase relations in the Mg-Ca-Si-Sr system for degradable biomaterials. Conference: 6th Symposium on Biodegradable Metals in Maratea, Italy. August 2014.

29. **Inge Bellemans**, Kim Verbeken, Nico Vervliet, Nele Moelans, Lieven De Lathauwer. Multi-component multi-phase field model combined with tensorial decomposition. VSC Users Day, November 30, 2015, University of Antwerp (Campus Drie Eiken), Belgium.
30. **Juan Guillermo Santos Macias**, Andrea Gil Santos, Nele Moelans, Omer Van der Biest. Influence of the grain size and phase content on the mechanical behavior of magnesium alloys for biodegradable implants. Gravity casting and SPS manufactured. Junior Euromat 2016, July 10-14, Lausanne.

## Dissertations

1. Master thesis: Calculation of phase diagrams for lead-free solder alloys based on Bi-In-Sn-Zn, June 2002.
2. PhD.-thesis: Phase-field simulations of grain growth in materials containing second-phase particles, May 2006.

## Internal Reports

1. Vanherpe, L., Moelans, N., Blanpain, B., Vandewalle, S. (2007). A bounding box algorithm for three-dimensional phase field simulations of microstructural evolution in polycrystalline materials. TW Reports, TW494, 14 pp: K.U.Leuven, Department of Computer Science.
2. Vanherpe, L., Moelans, N., Blanpain, B., Vandewalle, S. (2009). Pinning effect of spheroid second-phase particles on grain growth studied by three-dimensional phase field simulations. TW Reports, TW555, 21 pp: KU Leuven, Department of Computer Science.

## Promoter of completed PhD dissertations

1. Jeroen Heulens. Isothermal crystallization of metallurgical slags. Phase field simulations combined with in situ experiments. November 2011.
2. Yann Eichhammer. Thermodynamic and kinetic description of nanowires and nanowires growth. February 2012.
3. Hamed Ravash. 3D phase-field simulations of sintering and coarsening in polycrystalline multi-phase materials. November 2014.
4. Durga Ananthanarayan. Development of an elastoplastic phase-field model for multi-phase systems. March 2015.
5. Yuanyuan Guan. Development of a method to determine the solubility ranges of intermetallic compounds in metal-metal connections. November 2015.
6. Evelien De Wilde. Methodology Development and Experimental Determination of the Origin of Sticking Copper Droplets in Pyrometallurgical Slags. December 2015.
7. Jingjing Liu. In-situ observation and phase-field simulation of crystallization and dissolution phenomena in CaO-Al<sub>2</sub>O<sub>3</sub>-SiO<sub>2</sub> slags. August 2016.

8. Andrea Isabel Gil Santos. Phase diagram assessment and alloy characterization of ternary Mg rich Mg-Si-Ca and Mg-Si-Sr alloys for biomedical applications. May 9, 2017.
9. Inge Bellemans (U Ghent). Metal Droplet Entrainment by Solid Particles in Slags: A Combined Phase Field-Experimental Approach. May 24, 2017.
10. Nabi Nabiollahi (Imec). Processing induced changes of mechanical stresses in and near Cu Through Silicon Vias (TSVs): A Finite Element Modelling Study. December 14, 2017.