

COST

Domain Committee "Materials, Physical and Nanosciences"

COST Action P19

Start Date 02/02/2006

End Date 01/2/2010

Multiscale Modelling of Materials

FINAL EVALUATION REPORT

This Report stems from the relevant Domain Committee.

It contains four parts:

- I. Management Report prepared by the COST Office/Grant Holder*
- II. Scientific Report prepared by the Chair of the Management Committee of the Action.*
- III. Evaluation Report prepared by the "ad hoc" Evaluation Panel, established by the Domain Committee, and edited by the COST Office.*
- IV. DC General Assessment prepared by the Domain Committee*

Appendices:

Confidentiality: the documents will be made available to the public via the COST Action web page except for chapter *II.D. Self evaluation* and *III. Evaluation Report*.

Executive summary of the Scientific Report (max.250 words):

Multiscale modelling is a relatively new field of research which has in a short time had a significant impact on many scientific and engineering disciplines.

The Cost Action 19 was divided into four groups working on multiscale modelling of materials. They included: mechanical properties, phase transitions and chemical reactions, magnetic materials, and hybrid simulation methods. The action made great strides in its overall aim of developing methods to aid our understanding of material behaviour at different time and length scales, ranging from the atomic level, described using quantum mechanics, to macroscopic properties. The main emphasis of the action has been on 'hard' materials; however, one of the working groups concentrated on soft materials, hence providing a link towards actions working in that area.

The Cost action 19 has significantly contributed to the advancement of the multiscale modelling through fundamental theoretical and computational research, some of which can be considered to be at the forefront of the field. In addition the action has proved highly effective in providing the European researchers with a common platform for exchange of researchers and collaborations.

I. Management Report prepared by the COST Office/Grant Holder

I.A. COST Action Fact Sheet

Action P19 Fact Sheet

Title

Multiscale modelling of materials

Contacts

MC Chair	Science Officer:	Administrative Officer:
Prof. Matti ALATALO Lappeenranta University of Technology Lappeenranta Department of Electrical Engineering, P.O. Box 20 53851 Lappeenranta Finland Matti.Alatalo@lut.fi	Dr Caroline WHELAN COST Office caroline.whelan@cost.eu +32 2 533 38 14	Ms Marie-Eve HASTIR COST Office marie-eve.hastir@cost.eu +32 2 533 38 45

Details

Draft Mou: 303/05	Mou: 211/06
Start of Action: 02/02/2006	Entry into force: 18/01/2006
End of Action: 01/02/2010	CSO approval date: 14/06/2005

Objectives

The first meeting of the Management Committee took place on 2 February 2006 at the COST-Office in Brussels. The main objective of the Action is to increase the basic knowledge on technologically important materials and processes of their treatments and to provide a scientific basis for improving their macroscopic properties.

Parties

Country	Date	Country	Date	Country	Date	Country	Date
Austria	28/03/2006	Belgium	11/01/2006	Bulgaria	17/11/2006	Czech Republic	27/04/2006
Finland	11/01/2006	France	05/04/2006	Germany	18/01/2006	Greece	24/10/2007
Hungary	21/12/2006	Israel	29/01/2007	Lithuania	27/06/2008	Norway	09/03/2006
Poland	11/01/2006	Portugal	18/09/2006	Spain	18/01/2006	Sweden	21/06/2006
Switzerland	19/01/2006	United Kingdom	19/01/2006				

Total: 18

Intentions to accept the MoU

Country	Date	Country	Date	Country	Date	Country	Date
Italy	N/A						

Total: 1

Participating Institutions from non-COST countries

New Zealand	AUT University
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Working Groups

- WG 1: Michael Finnis
- WG 2: Karsten Reuter
- WG 3: Josef Fidler
- WG 4: Guy Courbebaisse

Website

<http://www.ipm.cz/costp19/>

Participating Institutions from non-COST countries

New Zealand	AUT University
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I.B. Management Committee member list

Austria

Professor Franz Dieter FISCHER MC Member Institute of Mechanics Montanuniversitat Leoben Franz-Josef-Strasse 18 8700 Leoben Austria mechanik@unileoben.ac.at	Professor Josef FIDLER MC Member Institute of Solid State Physics Vienna University of Technology Wiedner Hauptstr. 8-10 1040 Wien Austria josef.fidler@tuwien.ac.at
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Belgium

Dr. Dirk LAMOEN MC Member University of Antwerp Groenenborgerlaan 171 2020 Antwerpen Belgium Dirk.Lamoen@ua.ac.be	Professor Marcel AUSLOOS MC Member SUPRATECS Faculte des Sciences Universite de Liege B5, Sart Tilman 4000 Liege Belgium marcel.ausloos@ulg.ac.be	Professor Marc HOU MC Substitute Unievrsite Libre de Bruxelles Laboratoire de Physique des Solides Irradies et des Nanostructures CP234, Bd du Triomphe 1050 Bruxelles Belgium mhou@ulb.ac.be
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Bulgaria	
<p>Mr Gueorgui VASSILEV</p> <p>MC Member</p> <p>University of Plovdiv, Faculty of chemistry Tsar Asen 24, No 24 4000 Plovdiv Bulgaria gpvassilev@excite.com</p>	<p>Dr Nikolay VITANOV</p> <p>MC Member</p> <p>Bulgarian Academy of Sciences Institute of Mechanics Acad. G. Bontchev Str., bl 4 1113 Sofia Bulgaria vitanov@imech.imbm.bas.bg</p>
<p>Ms Vanya GANDOVA</p> <p>MC Substitute Member</p> <p>Plovdiv university 24 Tsar Asen 4000 Plovdiv Bulgaria gandova_71@abv.bg</p>	

Czech Republic	
<p>Professor Mojmir SOB</p> <p>MC Member</p> <p>Institute of Physics of Materials Zizkova 22 616 62 Brno Czech Republic mojmir@ipm.cz</p>	<p>Dr Vaclav PAIDAR</p> <p>MC Substitute Member</p> <p>Czech Academy of Sciences Institute of Physics Na Slovance 2 18040 Prague Czech Republic paidar@fzu.cz</p>
<p>Dr Jiri SVOBODA</p> <p>MC Substitute Member</p> <p>Institute of Physics of Materials Zizkova 22 CZ-616 62 Brno Czech Republic svobj@ipm.cz</p>	

Finland	
<p>Professor Kai NORDLUND</p> <p>MC Member</p> <p>Accelerator Laboratory Faculty of Science University of Helsinki P.O. Box 43 (Pietari Kalmin katu 2) 00014 University of Helsinki Finland kai.nordlund@helsinki.fi</p>	<p>Professor Risto NIEMINEN</p> <p>MC Member</p> <p>COMP/Laboratory of Physics Helsinki University of Technology P.O. Box 1100 02150 Espoo Finland risto.nieminen@hut.fi</p>

France	
<p>Dr. Charlotte BECQUART</p> <p>MC Member</p> <p>LMPGMUMR 8517 Université des Sciences et Technologies de Lille I Batiment C6, 2eme etage, Université des Sciences et Technologies de Lille I 59655 Villeneuve d'Ascq cedex France charlotte.becquart@univ-lille1.fr</p>	<p>Dr. Guy COURBEBASSE</p> <p>MC Member</p> <p>CREATIS-LRMN UMR 5220 CNRS -U630 INSERM - UCBL - INSA LYON BAT Blaise Pascal, 7 av. Jean Capelle 69621 Villeurbanne France guy.courbebaisse@insa-lyon.fr</p>

Germany

Professor Peter GUMBSCH MC Member Max Planck Institute Fur Metallforschung Frankfurt Institut of Materials IWM Wohwstr. 11 79108 Freiburg Germany peter.gumbsch@iwf.fraunhofer.de	Dr. Karsten REUTER MC Member Max Planck Gesellschaft Fritz Haber Institut Faraday weg 4-6 14195 Berlin Germany reuter@fhi-berlin.mpg.de
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Greece

Professor Vassilios TSIANTOS
MC Member
Technological Educational Institute of Kavala
Mathematics Technological Applications
Ag. Loukas 65404
Kavala Greece
tsiantos@otenet.gr

Hungary

Dr. Ferenc KUN
MC Member
University of Debrecen Egyetem ter 1, P.O.Box 37. 4032
Debrecen Hungary
feri@ica1.uni-stuttgart.de

Israel

Professor Konstantin VOLOKH MC Member Civil and Environmental Engineering Technion - Israel Institute of Technology Civil and Environmental Engineering, Technion - Israel Institute of Technology 32000 Haifa Israel cvolokh@technion.ac.il	Professor Jay FINEBERG MC Member The Hebrew University of Jerusalem Jerusalem Israel jay@vms.huji.ac.il
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Italy	
Dr. Francesco MONTALENTI MC Member Universita di Milano-Bicocca N/A - Please update this record Milano Italy Francesco.Montalenti@unimib.it	Dr. Claudio SERPICO MC Member Universita di Napoli Federico II Via Claudio 21 80125 Napoli Italy serpico@unina.it

Lithuania	
Professor Donatas Rimantas VAISNORAS MC Member FACULTY OF PHYSICS AND TECHNOLOGYVILNIUS PEDAGOGICAL UNIVERSITY STUDENTU ST 39 08106 Vilnius Lithuania vaisnoras@vpu.lt	Dr. Jelena TAMULIENE MC Member Institute of Theoretical Physics and Astronomy of Vilnius University Research Group of Theoretical Molecular Electronics and spintronics Institute of Theoretical Physics & Astronomy of Vilnius University A. Gostauto 12 01108 Vilnius Lithuania gicevic@itpa.lt

Poland	
Dr. Tomasz WEJRZANOWSKI MC Member Faculty of Materials Science and Engineering Warsaw University of Technology Woloska 141 02-507 Warsaw Poland twejrzanowski@inmat.pw.edu.pl	Professor Adam KIEJNA MC Member Institute of Experimental Physics University of Wroclaw pl. Maxa Borna 9 50204 Wroclaw Poland kiejna@ifd.uni.wroc.pl

Portugal	
Dr. Antonio GASPAR DA CUNHA MC Member IPC - Institute of Polymers and Composites Engineering School University of Minho Campus de Azurem 4800-058 Guimaraes Portugal agc@dep.uminho.pt	

Spain	
Professor Jesus M. GONZALEZ MC Member Associated Unit ICMM - IMA Crtra. A-6 km 22.5 28230 Las Rozas Spain jesusmgonzalez@jesusmgonzalez.jazztel.es	Dr Oksana CHUBYKALO-FESENKO MC Substitute Member Instituto de Ciencia de Materiales de Madrid N/A - Please update this record Madrid Spain oksana@icmm.csic.es

Sweden

Dr. Niklas WELLANDER
MC Member
Swedish Defence Research Agency,
FOISensor Technology P.O. Box 1165 581 11
Linköping Sweden
niklas.wellander@foi.se

Switzerland

Professor Till VALLEE
MC Substitute
Bernese Fachhochschule Architektur,
Holz und Bau Pestalozzistrasse 20 3401
Burgdorf Switzerland
till.vallee@bfh.ch

United Kingdom

Professor Michael FINNIS MC Member Imperial College London Faculty of Natural Sciences London Department of Materials, Imperial College London, Exhibition Road SW7 2AZ London United Kingdom m.finnis@ic.ac.uk	Dr. Richard James NEEDS MC Member TCM Group Cavendish Laboratory Madingley Road CB3 0HE Cambridge United Kingdom rn11@cam.ac.uk
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Non-COST Participants**New Zealand**

Professor Darius SINGH AUT University darius.singh@aut.ac.nz	
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I.C. Overview activities and expenditure

Action P19 - budget from 02-juin-2006 to 31-mai-2010						
Generated on 20-janv-2012						
Meetings						
Meeting Type	Date	Place	Paid part	Cost	Status	Total
Management Committee	18-sept-2006	Freiburg (DE)	12	7521,64	Paid	
In conjunction with Workshop	24-sept-2006	Wroclaw (PL)	15	10684,11	Paid	
In conjunction with Workshop	05-févr-2007	Lyon (FR)	3	3010,58	Paid	
Working Group	07-juin-2007	Naples (IT)	11	6364,09	Paid	
Management Committee	11-juin-2007	Lappeenranta (FI)	14	12206,3	Paid	
In conjunction with Workshop	17-juin-2007	Stockholm (SE)	5	3770,09	Paid	
In conjunction with Workshop	05-sept-2007	Brussels (BE)	6	4228,67	Paid	
Working Group	09-oct-2007	Lausanne (CH)	2	376,22	Paid	
Mid-term Evaluation Confer	25-juin-2008	Brno (CZ)	24	19202,72	Paid	
Working Group	30-mars-2009	Lyon (FR)	4	1150,3	Paid	
Management Committee	07-mai-2009	Oulu (FI)	6	5896,95	Paid	
In conjunction with Workshop	07-déc-2009	Levi (FI)	8	5199,27	Paid	
Working Group	08-déc-2009	Konstanz (DE)	11	3877,35	Paid	
Working Group	10-déc-2009	Carouge (CH)	1	730,59	Paid	
Final Evaluation Conference	23-avr-2010	Helsinki (FI)	6	1863,59	Paid	
						86082,47

Workshops						
Title	Date	Place		Cost	Status	Total
Workshop on Multiscale mo	24-sept-2006	Wroclaw (PL)		1.500	Paid	
WG 3 meeting: Magnetic Ma	07-juin-2007	Naples (IT)		500	Paid	
Third Management Committ	11-juin-2007	Lappeenranta (FI)		1.740	Paid	
Working Groups 3 and 4	09-oct-2007	Lausanne (CH)		530	Paid	
Mid-Term Evaluation Confer	25-juin-2008	Brno (CZ)		2.850	Paid	
WG4 meeting	30-mars-2009	Lyon (FR)		400	Paid	
Fifth Management Committ	07-mai-2009	Oulu (FI)		1.150	Paid	
COST P19 Workshop	07-déc-2009	Levi (FI)		3.000	Paid	
COST MEETING WORKING GR	08-déc-2009	Konstanz (DE)		1.350	Paid	
Working Group 3-4	10-déc-2009	Carouge (CH)		1.000	Paid	
						14.020

General Support Grants						
Title	Date			Cost	Status	Total
General	17-nov-2006			2.000	Paid	
General	01-juil-2007			2.000	Paid	
General	01-janv-2009			2.000	Paid	
General	01-janv-2010			2.000	Paid	
						8.000
Honoraria						
Title	Date	Expert		Cost	Status	Total
Final MC & Evaluation Confe	23-avr-2010	ALIABADI FERRI		500	Paid	
						500
					Action Total	170089,47

II. Scientific Report prepared by the Chair of the Management Committee of the Action, describing results achieved during the Action operation in this period, in no more than 3 pages (the report is “cumulative”). All items listed in Sections A, B, and C, below, must be addressed.

II.A. Innovative networking

- *Innovative knowledge resulting from COST networking through the Action: The Action has brought together scientists working on different aspects of materials modelling. For example, the micromagnetic modelling has recently moved to a new level, combining the atomistic description of the origins of the magnetic phenomena and the meso- and macroscale modelling needed for state-of-the-art practical applications. This is highlighted in the attached report of the meeting of working group 3 in Constance in December 2009.*
- *Significant scientific breakthroughs as part of the COST Action: Please see the attached reports and lists of publication.*
- *Tangible medium term socio-economic impacts achieved or expected: Even though most of the work performed in the Action is strictly speaking basic research, several socio-economic impacts can be expected. Modelling of materials leads to innovations in materials technology as well as in other areas. As an example, the methods developed within the Action have recently been applied to the study of cerebral aneurysms. This is highlighted in the attached report of working group 4 meeting in Geneva, November-December 2009.*
- *Spin off of new EC RTD Framework Programme proposals/projects (some of the projects may have started before 2009, but are still in progress):*
 - *COST action MP0903*
 - *Collaborative research project PERFORM60*
 - *Collaborative research project GETMAT*
 - *KMM-NoE Network of Excellence*
- *Spin off of new National Programme proposals/projects:*
 - *Multiscale modelling of chemical processes, a collaborative research project funded by the Academy of Finland*

II.B. Inter-disciplinary networking

- *Additional knowledge obtained from working with other disciplines within the COST framework: During the year 2009, our Action was very active in organizing training schools together with other COST Actions. Speakers from P19 attended the joint training schools both in Oulu, Finland and Brasov, Romania, the themes of these schools being photocatalysis and supercapacitors and other future energy devices, respectively. Both schools were very fruitful and brought up new interdisciplinary ideas, not only for the students but also for the speakers who came from several different COST Actions.*
- *Evaluation of whether the level of inter-disciplinarity is sufficient to potentially provide scientific impact: Since the topic of the action is multiscale modelling of materials, it necessarily involved interdisciplinarity. Most of the Action members are physicists or materials scientists by background, yet many groups work in fields close to chemistry, engineering or even medicine (see the attached WG 4 report).*
- *Evaluation of whether the level of inter-disciplinarity is sufficient to potentially provide socio-economic impacts: As described above, the work in the Action is mostly interdisciplinary. Several research groups within the Action work on applied problems, the solutions of which will have direct or indirect socio-economic impacts. Many of the research groups involved in the Action also have close collaboration with the industry. As an example, the group at Lappeenranta University of Technology, lead by the MC Chair, is working on multiscale modelling of TiO₂ nanoclusters in close collaboration with Sachtleben Pigments. Moreover, several research groups belonging to the Action are working together with the steel industry in order to develop better steels for, e.g., the future fusion reactors.*

II.C. New networking

- *Additional new members joining the Action during its life: New members have kept on joining the Action in a steady pace during its lifetime. During the past year, though, few new members have appeared, which is most likely due to the fact that this is the last year of the Action and the potential new members may feel that it is too late for them to join at this stage.*
- *Total number of individual participants involved in the Action work: Since the size of the research groups tends to vary quite rapidly, the exact number is hard to give. Yet an estimate is 80-90 people. Out of this number, some 30-40% are Early Stage researchers and less than 40% are female.*
- *Involvement of Early Stage Researchers in the Action, in particular with respect to STSMs, networking activities, and Training Schools. In addition, justification should be provided if less than 4 STSMs were carried out during the year: During 2009, 14 STSMs have been performed. Most of the STSMs have been carried out by Early Stage Researchers. The MC has always had a strong commitment to the involvement of Early Stage Researchers, which is reflected both in the form of STSMs and active organization of Training schools (for this year's training school activities, see paragraph II B above).*
- *Involvement of researchers from outside of COST Countries: One research group, lead by Prof. Darius Singh has been officially appointed by the CSO during the Action. Prof. Singh has been actively involved, giving talks in our workshops and hosting an STSM. In addition, several invited speakers in the workshops and training schools organized by the Action come from non-COST countries.*
- *Advancement and promotion of scientific knowledge through publications and other outreach activities: The list of publications of the members of the Action is attached to this report. As for the other outreach activities, please see paragraphs II B describing the involvement in the joint training schools, which were part of the COST outreach effort. (Number of publications and other outreach activities that resulted from COST networking through the Action. Complete list should be given in an annex)*
- *Activities and projects with COST network colleagues: During the Action, several new links have been established within the Action. The past year, being the last one of the Action, may have been slightly less active in that sense, yet STSMs between groups, which did not collaborate earlier, have been performed.*
- *The capacity of the Action members to raise research funds: As can be seen in the list given in paragraph II A, the members of the Action have been active in applying, and also obtaining research funds from both the EU and national agencies. It should be noted that the list given is not exhaustive, but should rather be regarded as an example of the types of funding attracted.*

III. Previous scientific report(s)

II.A. Results achieved during the period February 2006 to January 2008

The kick-off meeting of the Action was held in Brussels February 2nd 2006. Representatives from 9 countries were present at the meeting. During the first year of the Action, its size has increased to 16 countries (13 signed, 3 intentions in February 2007). The Action comprises of four working groups (WG), which started formally at the beginning of the Action, yet began taking shape already by the time the Action was accepted by the CSO. New groups from several countries have been joining in the WG's the most active countries being Poland and Czech Republic, both having contributed to the Action with several accepted proposals. The second management committee (MC) meeting was held

in Freiburg, Germany September 18th 2006.

The theme of the Action, multiscale modelling of materials involves both method development and the use of existing multiscale methods. Progress has been made in both areas, the method development naturally requiring a longer time span. The leading European groups, many of which belong to the Action, are in the forefront of the multiscale modelling research in the world.

From the applications point of view, the WG's cover a wide range of materials physics such as the fracture of materials, surface reactions, micromagnetism and multiparticle diffusion problems in solids. The methods used and developed include first principles statistical mechanics, molecular dynamics using different approximations and their combinations, different Monte Carlo schemes, cellular automaton simulations, micromagnetic methods and Lattice Boltzmann models. During the first year of the Action, several groups involved have become aware of the approaches used by other members of the Action, which is a key step towards the combination of previously separate methods and the application of the existing methods to new problems.

The timetable set at the memorandum of understanding was kept well during the first year of the Action. The WG's have been taking shape and several informal WG meetings have been held in the context of the MC meetings, conferences and workshops. The first WG meeting supported by the Action was held by WG4 in Geneva, see the report attached. The first general workshop of the Action was actually held ahead of schedule, in September 2006. At the workshop, a panel discussion was held, addressing the state-of-the-art problems in the field and serving the purpose of increasing the coherence between the different WG's. Similar discussions will be an important part of future workshops and WG meetings as well. One of the key things emphasized in the panel discussion was the need for international collaboration, combining both computational and human resources. The latter aspect is realized in collaborations such as the present Action; the former has been addressed in discussions between the Action members and representatives of national and European supercomputer centers.

From the very beginning of the Action, the MC has agreed to strongly support young scientists. Therefore, most of the STSM's have been performed by young graduate students or postdocs. During the visits, new computational methods have been learnt by

the young scientists, thus facilitating the diffusion of information between groups. We also encourage young scientists to give talks at the workshops supported by the Action. This has already led to several useful contacts and better integration of the working groups.

During its second year, the Action kept on growing and several new groups and countries joined in. The third MC meeting was held in Lappeenranta, Finland, June 11th 2007, where in addition to the normal MC matters a presentation by Klaus Lindberg, a representative of the Finnish IT centre for science CSC was given, addressing the European infrastructure for computational science. This infrastructure is very important from the point of view of our Action, which concentrates on computational modelling. In the context of the MC meeting, we organized a training school, which, even though not formally supported by the Action (see Section II C below), was attended by students from several member countries.

During the year 2007 no major workshops were organized by the Action, yet we supported three workshops and conferences (see Section II B), which were attended by several members of the Action. 9 STSM's were performed, the emphasis being again on supporting the research and networking of young scientists. The activities of the four working groups are briefly summarized as follows:

Working Group 1 (Mike Finnis, UK)

Two STSM visits were performed in October 2007: Ms. M. Materska, Jagellonian University, Poland, visited Dr. V. Pierron-Bohnes, IPCMS, Strasbourg, France and M. Cak from Brno, Czech Republic visited the group of Prof. Peter Gumbsch at the Fraunhofer Institute in Freiburg, Germany. An informal group meeting was held during the MC meeting and training school in Lappeenranta, Finland. The WG members participated in the workshops supported by the Action and Mike Finnis and Michael Moseler gave lectures at the training school in Lappeenranta, Finland.

Working Group 2 (Karsten Reuter, GE)

A few new groups joined the WG during the year 2007. 3 STSM's were performed between the participating groups. An informal group meeting was held during the MC meeting and training school in Lappeenranta, Finland. The WG organized a joint COST/CECAM workshop in Lyon (see Section II B), where several group members met; the final report of the workshop is attached.

Working Group 3 (Josef Fidler, AU)

This annual report describes the achievements during the year 2007 to establish an European collaboration on multiscale modelling in magnetic materials. The main objective of the working group WG3 (magnetic materials) is to lay the foundations for several active and exciting research areas for collaborations dealing with modelling the intrinsic properties and the complex behaviour of magnetic materials, and spanning length scales from the atomic level to the continuum and picoseconds to long time stability. The research activities should combine the modelling of intrinsic magnetic properties on the atomistic level and hysteresis properties including switching modes and times on mesoscopic level together with the functional behaviour of magnetic devices on the macroscopic level, such as recording devices, spintronic, magneto-elastic sensors, biomedical devices, etc.

The one-day working group meeting of WG3 (magnetic materials) was held on June 7th, 2007 at the University of Naples, Italy. Among the 12 invited speakers the topics reached from ab-initio calculations of intrinsic magnetic properties to the modelling of the magnetization reversal processes by micromagnetic simulations. The possibilities how to combine the various length and time scales incorporated in magnetic problems have been discussed.

Two STSM's have been granted during 2007 to intensify the collaboration between WG3 partners:

-) Gino Hrkac (University of Sheffield, UK) visited the Vienna University of Technology (D. Suess), from 19 Nov 2007 to 5 Dec 2007.*
-) Unai Atxitia (Instituto Ciencia Materiales Madrid ICMM-CSIC, Spain) visited the University of York (R. Chantrell) from 25 Nov 2007 to 9 Dec. 2007.*

At the moment the working group consists of about twenty active partners from nine countries. The collaboration between the working group partners will be strengthened by future STSM's.

Partner groups of WG3 of the COST Action P19 (status: 30-June-2007):

Giorgio Bertotti, INRIM, - Istituto Nazionale di Ricerca Metrologica, Torino, Italy, (g.bertotti@inrim.it)

Roy Chantrell, University of York, UK (rc502@york.ac.uk)

Luis Lopez Diaz, University of Salamanca, Spain, (lld@usal.es)

Manfred Faehnle, Max-Planck Institut fuer Metallforschung Stuttgart, Germany, (faehn@physix.mpi-stuttgart.mpg.de)

Hans Fangohr, University of Southampton, UK, (fangohr@soton.ac.uk)

Oksana Fesenko Chubykalo, CSIC, Madrid, Spain, (oksana@icmm.csic.es)

Jesus M. Gonzalez, CSIC, Madrid, Spain, (jesus.m.gonzalez@icmm.csic.es)

Oscar Iglesias, Universitat de Barcelona, Spain, (oscar@ffn.ub.es)

Hamid Kachkachi, Universite de Versailles St. Quentin, France, (hamid.kachkachi@physique.uvsq.fr)

Josef Kudrnovsky, Academy of Sciences of the Czech Republic, Praha, (kudrnov@fzu.cz)

Krzysztof M. Lebecki, Institute of Physics, Polish Academy of Sciences, Warsaw, Poland (lebecki@ifpan.edu.pl)

Jim Miles, University of Manchester, UK, (Jim.Miles@manchester.ac.uk)

Jacques Miltat, Universite Paris XI Orsay, France, (miltat@lps.u-psud.fr)

Ulrich Nowak, Univeristy of York, UK, (un500@york.ac.uk)

T. Schrefl, University of Sheffield, UK, (t.schrefl@sheffield.ac.uk)

Claudio Serpico, Università di Napoli "Federico II", Italy, (serpico@unina.it)

Dieter Suess, Vienna University of Technology, Austria, (dieter.suess@tuwien.ac.at)

Laszlo Szunyogh, Budapest University of Technology and Economics, Hungary, (szunyogh@heisenberg.phy.bme.hu)

Vassilios Tsiantos, Democritus University of Thrace, Ksanthi, Greece (tsiantos@otenet.gr)

Peter Weinberger, Center for Computational Materials Science, TU Vienna, Austria, (pw@cms.tuwien.ac.at)

Working Group 4 (Guy Courbebaisse, FR)

** Participation to the summer school in Lappeenranta, June 11th, 2007.*

** WG4 workshops in Lausanne October 9th, 2007.*

** CPC 2007 Congress – Brussels: Organisation of the session Lattice Boltzmann and conferences.*

The most important event during the year 2008 was the mid-term conference, held in Brno, Czech Republic in June 25-28. In the talks and subsequent discussions, several interesting ideas were presented. Perhaps most importantly, the interplay between the academia and the industry was emphasized in several talks. It is therefore obvious that the topics of the Action are finding important applications and that there is a clear need for multiscale modelling of material also outside the physics and materials science

community. Another highlight of the conference was the decision to build up a database of programs used in multiscale modelling of materials. The work is in progress to establish such a database, which without doubt will be useful for both scientists working inside the multiscale modelling community and others, interested in using the methods used and developed in the Action. The fourth MC meeting of the Action was held in the context of the conference. Informal WG meetings were also held.

The activities of the four working groups during 2008 can be summarized as follows:

Working group 1, Michael Finnis

WG1 Co-Organised Symposium G – “Morphology and dynamics of nanostructure and disordered materials via atomic-scale modeling” at EMRS Fall Meeting in Warsaw, 15-19 Sept. 2008.

The conference contributions listed in the enclosed list of publications indicate the level of dissemination in this working group.

Moreover, 1 STSM was performed within WG1 during the year 2008.

Working group 2, Karsten Reuter

No official WG meetings were held during the year. However, several WG members participated the mid-term conference in Brno and had informal discussions there. An invited talk in the mid-term conference was given by Karsten Reuter. Two STSMs were performed. The list of publications can be found at the combined publication list of the Action.

Working group 3, Josef Fidler

This annual report describes the achievements during the year 2008 to continue the European collaboration on multiscale modelling in magnetic materials. The main objective of the working group WG3 (magnetic materials) has been laid on the expansion of several active and exciting research areas for collaborations dealing with modelling the intrinsic properties and the complex behaviour of magnetic materials, and spanning length scales from the atomic level to the continuum and picoseconds to long time stability. The research activities of the working group partners have combined the modelling of intrinsic magnetic properties on the atomistic level and hysteresis properties including switching modes and times on mesoscopic level together with the functional behaviour of magnetic

devices on the macroscopic level, such as recording devices, spintronic, magneto-elastic sensors, biomedical devices, etc.

The multiscale aspect of the research of WG3 partners is reflected by the contributions at the mid-term Conference of the COST Action on "Multiscale Modelling of Materials", where three invited talks have shown results and progress from ab-initio calculations of intrinsic magnetic properties to the modelling of the magnetization reversal processes by micromagnetic simulations. The possibilities how to combine the various length and time scales incorporated in magnetic problems have been discussed:

-) L. Szunyogh, L. Udvardi, B. Lazarovits, A. Antal, B. Újfalussy, P. Weinberger, "Magnetic Structure of Thin Films and Finite Nanoparticles from First Principles"
-) O. Chubykalo-Fesenko, U. Atxitia, N. Kazantseva, D. Hinzke, U. Nowak, R.W. Chantrell: "Modelling of Fast Magnetization Dynamics in FePt: from Ab-Initio to Micromagnetic Approach"
-) T. Schrefl, G. Hrkac, A. Goncharov, "Design of Magnetic Materials and Devices Using Finite Element Micromagnetics"

Three STSM's have been granted during 2008 to intensify the collaboration between WG3 partners:

-) Jerome Jackson (University of York, UK) visited the Budapest University of Technology and Economics, HU (László Szunyogh,) from 3 to 7 March 2008.

Topic: Simulation of FM/AFM multilayers

-) Richard Evans, (University of York, UK) has been visiting Instituto de Ciencia de Materiales de Madrid ES (Oksana Chubykalo-Fesenko), in Dec.2008/Jan. 2009.

Topic: Atomistic Simulation of Exchange Bias and Surface Anisotropy in Magnetic Nanoparticles

-) Thomas Ostler, (University of York, UK) has been visiting Instituto de Ciencia de Materiales de Madrid ES (Oksana Chubykalo-Fesenko), in Dec.2008/Jan. 2009.

Topic: Atomistic Simulation of Rare Earth Doped Magnetic Alloys

At the moment the working group consists of more than twenty active partners from nine countries. The collaboration between the working group partners will be strengthened by future STSM's.

Working group 4, Guy Courbebaisse

The Working Group 4 is dynamic moving in several directions with a common thread: the method of Lattice Boltzmann.

- In Lausanne (Switzerland) is a detailed study of the boundary conditions in the codes of Boltzmann behind the research. Also free software is now available and provides a common development platform for developers and users of this method

<http://www.lbmethod.org/openlb/>

In addition, the scope of work involves numerical simulation of viscoelastic materials.

- In Geneva (Switzerland) and in Lyon (France), the work concerns a multiphase Boltzmann method. The field of application involves the simulation of thrombosis for giant aneurysms of the brain. The ultimate goal is to classify aneurysms are at risk or not.

-In Zurich (Switzerland), the goal concerns optimization of the entropic lattice Boltzmann method.

A non-exhaustive list of publications is joined at the end of this report.

The WG4 forthcoming deadlines are as follows:

-One WG4 meeting will be organised (if possible) in February in Lyon or Lausanne

-One STSM for Guy Courbebaisse, during 2 weeks in April or May 2009: a scientific mission is planned in April 2009 in the lab of EPFL LIN led by Professor Michel Deville.

- One STSM for CREATIS's PhD student, during 1 month in July 2009: a scientific mission is planned in April 2009 in the lab of CUI – Geneva University led by Professor Bastien Chopard.

Result of research:

CREATIS lab is a partner of the VPH NOE consortium dedicated to numerical simulation and investigation of the human body as a single complex system.

Project in preparation for 2009:

A STREP project in the 7FP framework – 4th call / VPH, is envisaged with Geneva University, EPFL Lausanne, and others partners. The deadline is probably April 2009.

Project for COST P19 consortium:

To continue to develop the consortium COST P19, a future project in the field of numerical simulation methods seems appropriate. Indeed, it seems that in the European research projects seems a pitfall the sharing of simulation methods.

In this context, following the COST P19 could be considered as a NOE (7 FP) dedicated to numerical simulation methods and their coupling. This project would be generic enough to serve as a platform to STREP or others projects, since all fields of applications are concerned.

II.B. Dissemination of results

- The list of publications by the members of the Action is enclosed as a separate attachment.
- The first workshop of the Action, titled 'Workshop on multiscale modelling of extended defects and phase transformations at material interfaces', organized by Adam Kiejna and Mojmir Sob was held in Wroclaw September 24-26 2006. The programme and list of participants is attached.
- *During the year 2007 we supported the following workshops:*
 - *Multiscale Approaches to Nanomechanics, Lyon, France, February 5-7 2007. The final report, including the program and list of participants is attached.*
 - *Multiscale approach to alloys: Advances and challenges, Sigtuna, Sweden, June 17-19 2007. The programme of the workshop is attached.*
- The mid-term conference of the Action, titled 'Midterm conference on Multiscale Modelling of Materials' was held in Brno, Czech Republic, June 25-28 2008, organized by Mojmir Sob. The scientific report of the conference is attached.
- The web page of the Action is maintained by the group of Prof. Mojmir Sob in Czech Republic, the address of the page is <http://www.ipm.cz/costp19/>. It contains description of the Action, news on the upcoming events and links to the official Action web page at COST and other relevant COST pages.
- *Scientific and Technical Cooperation*

Individual groups and institutions belonging to the Action have established contacts to several scientific institutes and research programmes. Consortia suitable for the 7th framework programme have been formed both inside the Action and with outside partners, also involving industry.
- *Transfer of results*

Discussions have been conducted with several industrial companies, many of

which have shown interest to the topics of the Action. Groups belonging to the Action have started collaborative projects involving industrial partners.

- *Contacts in the ERA*

Even though the Action as a whole does not have formal contacts with other R&D programmes, many of its members are involved in such activities. For example, some of the MC members belong to other COST Actions as well. Moreover, some of the Action members are active in ESF networks such as the Psi-k network and KMM-NoE, the activities of which are closely related to the Action. *The abovementioned workshops have been organized together with the ESF networks Psi-k and SimBioMa, and CECAM.*

IV. DC General Assessment prepared by the Domain Committee

The DC agreed on the following General Assessment and suggested comment:

'COST Action P19 was approved with the main objective to increase knowledge and developing methods for understanding materials at different time and length scales.

It effectively created a platform for scientific collaboration and exchange of researchers to work in an effective way to contribute to the advancement of multiscale modelling through fundamental theoretical and computational research. The main focus was on technologically important materials and processes of their treatments and provide a scientific basis for improving their macroscopic properties. Throughout the whole community (supported by 18 COST countries and one non-cost country) could be reached interesting results with significant impact in many scientific and engineering fields. Significant highlights include for example

- the modelling of Fe-Cr(-Ni) steels*
- the calculation of cleavage energies in order to understand the mechanical properties of duplex steels*
- the modelling of dislocations using molecular dynamics with forces derived from quantum mechanics.*
- the design of magnetic materials and devices using finite element micromagnetics.*

The Action came to results of major importance in all the areas of research it covered by the 4 working groups: namely in mechanical properties, Phase transitions and chemical reactions, Magnetic materials, and Hybrid simulation methods. The scientific achievements and main outcomes of the Action P19 contributed to establishing working European networking structure and strengthening European leadership in the field multiscale modelling of materials.

The scientific outcome of the Action has been disseminated in over 200 publications from which 1/3 are joint publications.

The Action P19 has been beneficial to those who have taken part - a large number of people have been involved and involvement of researchers from outside COST countries has been strong. Action P19 has promoted multiscale modelling of materials and had a good impact on the training of young researchers through a number of summer schools, STSM and conferences with support of COST.'