

VERY PRELIMINARY PROGRAM FOR
ATOMCAD NETWORK MEETING AT
THE
MATERIALS-PHYSICS LAB IN
GÖTEBORG

Premeeting Session - discussing the SiC materials research

Place:	Time:	Date:
Soliden	9:00-12:00	Thursday, February 6, 2003.
9:00-12:00	Focused Session: SiC research interaction ; group discussions.	Elwira Wachowicz and Eleni Ziambaras <i>Unconfirmed</i>

Opening Session - Discussing the ATOMCAD research network

Place:	Time:	Date:
Soliden	12:00-19:00	Thursday, February 6, 2003.
12:00-14:00	Extended welcome and buffet at the Gothenburg lab	Camilla Eriksson , Per Hyldgaard and Bengt Lundqvist Confirmed
14:00-14:30	Presentation: <i>Barcelona! Barcelona! Activities at the CSIC</i>	
Riccardo Rurali and Jose Rebollo	Confirmed	
15:00-15:30	COFFEE BREAK	
	Confirmed	
16:00-17:00	Discussion: <i>Lessons of the Paris meeing</i>	
Andreas Larsson Chairman	Confirmed	
17:00-18:00	Discussion: <i>How to develop the ATOMCAD network for young researchers</i>	
Round table discussion	<i>Confirmed</i>	
18:00-18:30	Presentation: <i>ATOMCAD at LAAS - invitation from Toulouse</i>	

Leonard Jeloica and Mehdi Djafara-Rouhani	Confirmed		
18:30-19:00	Presentation: Make it a SigmaPlus day in Toulouse	Daniel Hill	Confirmed
19:30-21:00	Dining at restaurant Lagom		Confirmed

Meeting and Interaction Session

Place: [Soliden](#) **Time:** 9:00-12:00 **Date:** Friday, February 7, 2003.

9:00-10:30	Exchange: Official ATOMCAD meeting	ATOMCAD seniors	Confirmed
	Group work: Some Chalmers Research tools	ATOMCAD postdocs	Confirmed
10:30-11:00	COFFEE BREAK		
	Confirmed		
11:00-11:30	Topical Focus: The SiC materials ; Presentation and discussions	ATOMCAD/Chalmers participants	<i>Interest confirmed</i>
	Topical Focus: Kinetic Monte Carlo Modeling ; Presentation and discussions	ATOMCAD/Chalmers participants	<i>Interest confirmed</i>
11:30-12:00	Presentation: Activities at CEA and Collaborations in Paris	Nicolas Richard	Confirmed
12:00-12:30	Presentation: Limerics and Activities at the NMRC in Cork	Andreas Larsson	Confirmed
12:30-14:00	Lunch at the Chalmers Hyllan		Confirmed

Presentation and Discussion Session

Place: [Soliden](#) **Time:** 14:00-17:00 **Date:** Friday, February 7, 2003.

14:00-15:00	Discussion: Creating the ATOMCAD science exchange	Discussion and development	
	Confirmed		
15:00-16:30	COFFEE SHOP (coffee, cake, and presentations): Visit the Chalmers Materials and Surface Theory group	Part of the MST group , including Elwira Wachowicz , Per Hyltdgaard , and Bengt I Lundqvist	Confirmed
17:00-24:00	A night on the Gothenburg town (Dining, Concert, Art, and/or Jazz)		Quite Voluntary

Communication and Collaboration Session

Place: [Soliden](#) **Time:** 9:00-12:00 **Date:** Saturday, February 8, 2003.

9:00-11:00	Group work: A) What defines a good ATOMCAD collaboration?	ATOMCAD participants	Confirmed
	Group work: B) How do we integrate our ATOMCAD Research tools	ATOMCAD exchange, Daniel Hill, coordinator	Confirmed
11:00-11:30	Topical Focus: Oxidation and oxides ; Brief presentations	Elsebeth Schröder , ATOMCAD/Chalmers participants	<i>Interest confirmed</i>
	Topical Focus: Sample topics discussion ; Brief presentations	ATOMCAD/Chalmers participants	<i>Unconfirmed</i>
12:00-13:30	Buffet at fort Soliden		Confirmed

Conclusion Session

Place: [Soliden](#) **Time:** 13:30-18:00 **Date:** Saturday, February 8, 2003.

13:30-14:00	Topical Focus: Oxidation and oxides ; Discussion and interactions	ATOMCAD/Chalmers Participants	<i>Interest confirmed</i>
14:00-14:30	Topical Focus: SiC/Oxide behavior ; Discussion and interactions	ATOMCAD/Chalmers participants	<i>Interest confirmed</i>
14:30-15:00	Topical Focus: Sample topic discussion	ATOMCAD/Chalmers participants	<i>Unconfirmed</i>
15:00-15:30	COFFEE BREAK		
15:30-17:00	Confirmed Discussion: The ATOMCAD science exchange A) What defines a good ATOMCAD collaboration? B) How do we integrate our research tools? C) Summary	ATOMCAD participants	Confirmed
17:30-19:00	Relaxation		Recommended

19:00-23:00 [The ATOMCAD network dinner at Thörnströms kök](#)

Confirmed

Last updated 2003-02-05, [Per Hylgaard](#)

Participants : Jean-Paul Berhault (EU ATP officer), Mehdi Djafari Rouhani (LAAS/LPST), Alain Estève (LAAS), Daniel Hill (SIGMAPLUS), Per Hylgaard (Chalmers Univ.), Léonard Jeloica (LAAS), Andreas Larsson (NMRC), Bengt Lundqvist (Chalmers Univ.), Jose Rebollo (CNM), Nicolas Richard (CEA), Riccardo Rurali (CNM), Elsebeth Schröder (Chalmers Univ.), Elwira Wachowicz (Chalmers Univ.), Eleni Ziambaras (Chalmers Univ.)

The main purpose of the meeting was to reinforce networking and training activities

I - Research activities

It was reminded that research activities in collaboration between several partners were running inside the network.

- SiO₂ thermal growth involving CEA and LAAS/LPST with the near future perspective of determining different oxygen migration barriers : direct dimer to dimer, direct back-bond to back-bond, back-bond to back-bond via a strand position,
- High -k material deposition involving NMRC and LAAS/LPST. Five molecular states with their corresponding energies have been obtained for each of the three precursor molecules : HfCl₄, ZrCl₄, Al(CH₃)₃, for the first half reaction of the ALD process. Work is in progress for the second half reaction
- SiC material processing involving CNM, CUT and LAAS. The processes of diffusion for doping the material and the gate oxidation are of particular interest, but SiC – metal interfaces, such as SiC-Ni and SiC-Al, and the mechanisms of graphite precipitation in SiC have also been investigated.

Among other research activities, the following could be highlighted :

- At CEA
 - Mesoscopic approach in the silicon oxide electric transport using TRAPOX package

- Electronic properties of neutral and charged defects in amorphous SiO₂ : Si and O vacancies and interstitials using 5 Tflops computers with 2560 processors
- At CUT
 - Shape of the islands during Kinetic Monte Carlo deposition of Al/Al(111)
 - Effect of lateral atomic interactions in NO oxidation on Pt(111) surfaces. This allows the determination of oxidation efficiency as a function of surface coverage
 - Investigation of Thermodynamic phase stability, mechanical properties (Young Modulus and Poisson ratio anisotropy), phonon spectra
 - Mg oxidation using Monte Carlo simulated annealing. An interaction potential grid is determined from ab initio calculations
- At NMRC
 - Electronic structure of the excited states of molecules using Monte Carlo Configuration Interaction method and the COLUMBUS software package as the interface

II - Networking

New Recruitments

- Daniel HILL HAS JOINED SIGMAPLUS as a post doc in Dec. 2002 to set up a software platform for cooperative remote work,
- Ahmed DKHISSI has joined LAAS-CNRS as a post doc in January 2003 to investigate the functional properties of semiconductor surfaces exposed to molecules in gas or liquid phase
- There is still one vacant position at CEA and one vacant position at CUT. It is very likely that the position at CEA be transferred to LAAS because of lengthy procedures needed for the admission of foreign researchers into CEA

Secondment of Young Researchers

- Andreas Larsson to CNM in April 2003 to work on SIESTA package
- Elwira Wachowicz to LAAS in April 2003 to work on OXCAD package

- Andreas Larsson to Chalmers Univ. in May 2003 to work on DACAPO
- Riccardo Rurali to LAAS in March 2003 to work on OXCAD
- Leonardo Jeloica to Milano in March 2003 to set up a collaboration with INFM
- Ahmed Dkhissi to CUT in Sept. 2003 to work on Van der Waals interaction using ab initio methods
- Ahmed Dkhissi to NMRC in May 2003 to work on biological applications
- Daniel Hill to all places to set up the software platform

Participation of Young Researchers to conferences

- Andreas Larsson to Irish Atomistic Simulations, Dec. 16th – 17th 2002, Dublin
- Andreas Larsson to American Chemical Society Meeting, March 23rd – 27th 2003, New Orleans, USA
- Andreas Larsson to Physics Spring School in Toulouse, Apr. 7th – 11th 2003, Toulouse
- Leonard Jeloica to GDR Nanoelectronique, Jan. 29th – 31st 2003, Grenoble
- Leonard Jeloica to Journées Simulation Numeriques, May 2003, Paris
- Leonard Jeloica to E-MRS spring meeting, June 10th – 13th 2003, Strasbourg
- Ahmed Dkhissi to Journées Simulation Numeriques, May 2003, Paris
- Elwira Wachowicz to E-MRS spring meeting, June 10th – 13th 2003, Strasbourg
- Elwira Wachowicz Physics Spring School in Toulouse, Apr. 7th – 11th 2003, Toulouse
- Daniel Hill to Microscopy of Semiconductor Materials, May 2003, Cambridge
- Daniel Hill to Micro-technologies for the new Millennium 2003 : Nanotechnologies, May 19th – 21st 2003, Canaries
- Daniel Hill for a training on software platforms (to be defined)

Set up of a cooperative platform

The set up of a software platform for cooperative work was one of the objectives of the ATOMCAD network. This task was in charge of SIGMAPLUS who has recently recruited Daniel Hill to perform this job. The general architecture of the platform could be made of a Graphical User Interface (GUI) which would be connected to each of the available software packages through an interpreter. Several GUI and common protocols have already been investigated and compared to each other by Daniel Hill. It seems that JAVA language is best suited for both GUI and interpreter applications.

To start with the programme, a limited set of software packages have been chosen. The choice has been made on the basis that all partners be represented. The chosen packages are :

- MCCI developed at NMRC
- OXCAD developed at CEA and LAAS
- DACAPO presently used at Chalmers Univ.
- SIESTA presently used at CNM
- TROCADERO presently used at CNM
- VIBRATOM developed at LPST
- SPARCC developed at LAA/LPST

The four top packages will constitute the first set. If, for some proprietary reasons, the package is not available for common use, we can go down the above list.

On the other hand, Daniel Hill is going to develop the necessary cooperative and security protocols to ensure proper operation of the platform. Once the feasibility of cooperative work through the platform is demonstrated, we will extend the platform to other available software packages. At the same time, we will have to set up rules for the use of packages by internal ATOMCAD partners and by external users.

Set up of a Newsgroup

In order to promote tightening the links between ATOMCAD partners, Daniel Hill suggests to set up a newsgroup acting as a discussion forum for ATOMCAD.

Training

- Organisation of “Physics Spring School in Toulouse : Modelling and simulation in Micro and Nano Technologies and Materials Engineering”, April 7th – 11th 2003, Toulouse. The school is open to Young Researchers from ATOMCAD and to external PhD students or junior researchers. The objective is to provide the basic ideas behind the atomic scale modelling and to show their application in different fields,
- A Master diploma entitled “Modelling for Materials and Physical Processes Engineering” is under preparation at the Univ. of Toulouse. We intend to give a European label to this Master degree. The courses should normally start on Sept. 2004. The students will be recruited among those having already performed the first year of a physics or Chemistry Master. The duration of the course is one

complete year including a four to six months period in industrial environment. The students will end up with a Master degree.

- A Master on Materials already exists at the Chalmers Univ. of Technology. 16 students are regularly registered at this Master which is open to European students through Erasmus programme. A "Materials Theory" course, equivalent of five cursus points, is already taught within this Master.

III – Perspectives within FP6

ATOMCAD has been at the origin of the NANOTOOL initiative. NANOTOOL "Nano scale science for multi scale materials and devices" is a Network of Excellence to be proposed to FP6 Priority 3 "Nanotechnologies, intelligent materials, new production processes" programme. The NoE gathers 11 already existing "Research and Training Networks" involved in this field, who have decided to join their effort to promote Nanoscience and Nanotechnologies in Europe. The consortium brings together 80 labs belonging to 61 European institutions with more than 250 researchers involved. An EoI has already been submitted in June 2002.

During the present meeting, the general organisation and chart of NANOTOOL were discussed before proposal to other partners. In particular, it was decided that ATOMCAD will actively participate, and eventually coordinate, two research programmes oriented on the "Design of Functional Surfaces for Biological and Biochemical Applications" and on the "Oxidation of Materials for Microelectronics Applications".