Interuniversity Attraction Poles (IAP)  
Phase VI  
2007 – 2011  

ANNEX I  
TO CONTRACT P6/42  

TECHNICAL SPECIFICATIONS : SECTION II  

Information on the partners  
to be completed by each network partner including the EU-partner(s)  

Title of the project : Quantum effects in clusters and nanowires  

Name of the partner : BOGAERTS Annemie  
Institution : Departement Chemie, PLASMANT, Universiteit Antwerpen
II. 1. PARTNER CONTACT DETAILS

PARTNER N° (consult the list in Section I of Annex I) * : P4

- Family Name : Bogaerts
- First Name : Annemie
- Title (Prof., Dr., … ) : Prof. Dr.
- Institution : Universiteit Antwerpen, PLASMANT
- Institution’s abbreviation : UA - PLASMANT
- Faculty/Department : Faculty of Sciences / Department of Chemistry
- Research Unit : PLASMANT
- Road/Street, n° : Universiteitsplein 1
- Post Code : 2610
- Town/City : Wilrijk
- Country : Belgium
- Tel : +32-3-820.23.77
- Tel secretariat : +32-3-820.23.41
- Fax : +32-3-820.23.76
- E-mail : Annemie.bogaerts@ua.ac.be
- Website : http://webhost.ua.ac.be/plasma or: www.ua.ac.be/plasmant

* For Belgian partners : P1 to P6
For EU-partner : EU
II. 2. STAFF MEMBERS WORKING ON THE PROJECT (paid and not paid by the IAP-budget)

<table>
<thead>
<tr>
<th>Staff</th>
<th>Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Professor</td>
<td>1</td>
</tr>
<tr>
<td>Senior scientist</td>
<td>0</td>
</tr>
<tr>
<td>Post-doc</td>
<td>5</td>
</tr>
<tr>
<td>PhD student</td>
<td>7</td>
</tr>
<tr>
<td>Researcher without PhD</td>
<td>0</td>
</tr>
<tr>
<td>Technician</td>
<td>1</td>
</tr>
<tr>
<td>Secretary</td>
<td>0</td>
</tr>
<tr>
<td>Other</td>
<td>1</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>15</strong></td>
</tr>
</tbody>
</table>
II. 3. SKILLS OF THE STAFF MEMBERS

Indicate the name, profile (professor, senior scientist, post-doctoral, PhD student, researcher without PhD, technician, secretary or other) and areas of skills (5 lines maximum) of the most important personnel currently working within the project's framework (paid or not paid by the IAP-budget).

1. Name: Annemie Bogaerts  
   Profile: Professor  
   Skills: Numerical modelling of plasmas, plasma-solid interaction and laser-solid interaction, used for analytical characterization of solid materials, and for materials technology (deposition of thin films, production of nanoparticles, …)

2. Name: Erik Neyts  
   Profile: Post-doctoral researcher  
   Skills: Molecular dynamics and fluid dynamics simulations of chemical vapour deposition (CVD) or plasma-CVD of thin films (carbon-based and metal-oxide films); study of nucleation mechanisms.

3. Name: Neyda Baguer  
   Profile: Post-doctoral researcher  
   Skills: Molecular dynamics simulations of deposition of thin metal-oxide films; study of nucleation mechanisms

4. Name: Dragana Petrovic  
   Profile: Post-doctoral researcher  
   Skills: Particle-in-cell – Monte Carlo collision simulations of magnetron discharges used for sputter-deposition of thin films.

5. Name: Violeta Georgieva  
   Profile: Post-doctoral researcher  
   Skills: Molecular dynamics simulations of deposition of thin metal-oxide films; study of nucleation mechanisms

6. Name: Davide Bleiner  
   Profile: Post-doctoral researcher  
   Skills: Study of laser-solid interaction (heating, melting, vaporization, splashing of molten material, explosive boiling) by numerical modelling, with the purpose of describing nanoparticle and micrometer particle (droplet) formation; fluid dynamics simulations of gas flow behaviour in laser ablation cells.

7. Name: David Autrique  
   Profile: Ph.D. student  
   Skills: Fluid dynamics modeling of laser-solid interaction (heating, melting, vaporization), vapour plume expansion and plasma formation, and nanoparticle formation by condensation in the expanding vapour plume.

8. Name: Tom Martens  
   Profile: Ph.D. student  
   Skills: Fluid model of dielectric barrier discharges for deposition of SiO₂ thin films.

9. Name: Ivan Kolev  
   Profile: Ph.D. student

10. Name: Evi Bultinck  
Profile: Ph.D. student  
Skills: PIC-MC simulations of a magnetron in argon/nitrogen or argon/oxygen mixtures, for the deposition of metal nitride or oxide layers.

11. Name: Maxie Eckert  
Profile: Ph.D. student  
Skills: Molecular dynamics simulations for the deposition of (ultra)nanocrystalline diamond thin films.

12. Name: Stefan Tinck  
Profile: Ph.D. student  
Skills: Hybrid Monte Carlo - fluid simulations of an inductively coupled plasma reactor used for plasma etching applications of Si and SiO₂.

13. Name: Marinko Marinkovic  
Profile: Ph.D. student  
Skills: Molecular dynamics simulations for the growth of carbon nanotubes by plasma deposition

14. Name: Rabyie Aydin  
Profile: M.Sc. student  
Skills: Molecular dynamics simulations for the deposition of diamond-like carbon thin films

15. Name: Luc Van’t dack  
Profile: Technician  
Skills: Administration, maintenance of the computers, organization of workshops.
II. 4. PUBLICATIONS

Give a list of the most relevant 5 to 10 recent publications in direct relation with the proposed research.

1) Laser ablation for analytical sampling: What can we learn from modeling?
2) Numerical investigation of particle formation mechanisms in silane discharges.
3) Modeling of the formation and transport of nanoparticles in silane plasmas.
4) Role of the thermophoretic force on the transport of nanoparticles in dusty silane plasmas.
5) Unraveling the deposition mechanisms in a-C:H thin film growth: a molecular dynamics study for the reaction behavior of C₃ and C₄H radicals with a-C:H surfaces.
6) Detailed modeling of hydrocarbon nanoparticle nucleation in acetylene discharges.
7) The effect of hydrogen on the growth of thin a-C:H films from thermal energy radicals.
8) Aromatic ring generation as a dust precursor in acetylene discharges.
9) Multiplicity and contiguity of ablation mechanisms in laser-assisted analytical micro-sampling.
10) Structure of multi-species charged-particles in a quadratic trap.
II. 5. INTERNATIONAL CONTACTS IN THE PROJECT’S RESEARCH DOMAIN

Mention the international contacts and the international networks to which the partner belongs within the context of the project.

The work on modelling of nanoparticle formation in silane and hydrocarbon-based plasmas is carried out in close collaboration with Prof. Dr. Wim Goedheer from the Institute of Plasma Physics “Rijnhuizen” (NL). (in total: 19 joint publications since 1995)

The work on molecular dynamics simulations of deposition of thin carbon-based films is performed in close collaboration with Prof. Dr. ir. Richard van de Sanden, from Eindhoven University of Technology (NL). (5 joint publications since 2004)

The work on nanoparticle formation as a result of laser-solid interaction (laser ablation) occurs partly in the framework of a Project of the Flemish Community: Bilateral Scientific and Technological Collaboration with China: “Numerical modelling of the interactions of femtosecond and nanosecond laser pulses with a solid and with plasma”; in collaboration with Prof. Yu Wei (Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, China).

The work on nanoparticle formation in laser ablation is also carried out in close collaboration with Prof. Dr. Akos Vertes from the George Washington University (US). Last year, prof. Vertes carried out a sabbatical stay of 3 months in Belgium, with a fellowship of the Royal Flemish Academy of Sciences, in a collaboration with our group and University of Leuven (Prof. Dr. Peter Lievens).
II. 6. CONTRACTS IN PROGRESS IN THE PROJECT'S RESEARCH DOMAIN

Give the list of research projects currently carried out in the field of the project with the duration and the funding source (Belgium's Federal Government, Communities and Regions or by the European Union,…).


3) 2005-2006: Project of the Flemish Community: Bilateral Scientific and Technological Collaboration with China: “Numerical modelling of the interactions of femtosecond and nanosecond laser pulses with a solid and with plasma”.


6) 2006-2008: IWT project: “Nucleation and durability of very thin CVD oxide films on steel and metallic coated steel”.

7) 2007-2010: FWO Research project: “Growth, characterisation and simulation of nanocrystalline and ultrananocrystalline PE-CVD diamond films ».
II. 7. WORKPACKAGES IN WHICH THE PARTNER IS PARTICIPATING

1. Workpackage number and title: 1: Metallic and oxide clusters
2. Workpackage number and title: 3: Semiconductor quantum dots and wires
3. Workpackage number and title: 5: Carbon nanotubes and related materials
II. 8. BUDGET (distribution per year) *

(in EURO, without decimals)

<table>
<thead>
<tr>
<th></th>
<th>2007</th>
<th>2008</th>
<th>2009</th>
<th>2010</th>
<th>2011</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Personnel</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
</tr>
<tr>
<td>Operating costs</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
</tr>
<tr>
<td>Equipment</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td></td>
<td>Not allowed</td>
</tr>
<tr>
<td>Overheads</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
</tr>
<tr>
<td>Subcontracting</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
</tr>
<tr>
<td>Subtotal</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
</tr>
<tr>
<td>EU 1 (name)</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
</tr>
<tr>
<td>EU 2 (name)</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
</tr>
<tr>
<td>EU 3 (name)</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
</tr>
<tr>
<td>EU 4 (name)</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
</tr>
<tr>
<td>Total</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
<td>0,00</td>
</tr>
</tbody>
</table>

* This table should not be completed by the European partner as his/her budget is mentioned in the budgetary table of the Belgian partner of the network responsible for the follow-up of the partnership.
- ** Personnel**: indexed gross remunerations; employer’s social contributions; statutory insurance costs as well as any other compensation or allocation legally due in addition to the salary; the reimbursements for PhD and postdoctoral grant holders (exempt from tax and benefiting from social security). Personnel costs must account for minimum 60% of the total budget attributed to each partner of the network. The costs for the tax-free PhD grants and postdoctoral grants may not account for more than 60% of the total personnel costs.

- ** Operating costs**: documentation; travel and accommodation; hosting of visiting foreign researchers; use of computing facilities; software; telecommunications; maintenance and operation of equipment and, more generally, consumables;.

- ** Equipment**: acquisition and installation of scientific and technical appliances and instruments, including IT equipment placed at the project’s disposal. Equipment cannot be asked for during the last year of the programme.

- ** Overheads**: general expenses of the institutions covering, on an inclusive basis, administrative, telephone, postal, maintenance, heating, electricity, rental, material depreciation and insurance costs. The total amount for this heading may not exceed 5% of total personnel and operating costs.

- ** Subcontracting**: costs incurred by a third party in order to perform tasks or provide services necessitating specific scientific or technical skills outside the normal framework of the institution’s activities. Each request for subcontracting needs a approval from the programme administrator.
II. 9. EQUIPMENT

Indicate the equipment (with an estimation of the cost) that will be purchased from the IAP-budget for the coming four years (2007-2010) and justify.
II. 10. SUBCONTRACTING

*To be completed only if subcontracting is foreseen.*

Describe and justify the tasks and/or services that will be provided by a third party.