WORKSHOP

The role of laboratory experiments in the characterisation of cosmic material

Bern, 8 – 12 May 2000

1. Background

The characterisation of cosmic dust and ice properties in different space environments represents one of the most interesting subjects of modern astrophysics. Thanks both to the improvement of ground-based observational methods and to the advent of space-born observatories (such as HST and ISO, in the past and present, and Planck-FIRST and SIRTF for the future) a wealth of new observational data become day by day available and give a more accurate view of the distribution of cosmic materials and their physico-chemical properties and evolution. The advent of 8 m class telescopes, such as VLT which has shown first light in 1998, will be a major tool to search for weak dust features in interstellar, circumstellar and interplanetary space. In this scenario, laboratory experiments play a central role. Several groups around the world place strong efforts on the production and characterisation of laboratory analogues of cosmic compounds and to simulate the astrophysical processes relevant in space. This approach supports, on a quantitative basis, the interpretation of observations.

Nevertheless, the interpretation of observations is far from being complete. Actually, several long standing open problems remain unsolved and new key questions await answers. In particular, the attribution of several typical dust and ice features, observed in interstellar medium, in circumstellar environment and in comets, is not yet clear. Moreover, it is clear that materials evolve in space due to physical and chemical conditions in the local environment. Actually, the life cycle of interstellar dust is bound to the evolution of stars in the Galaxy. The formation of complex molecules occurs already during the evolutionary cycle of interstellar icy grains which are originally formed in dark clouds. The link between processes in dark embedded clouds and comets seems to be evident and studies on the connection between interstellar, cometary and meteoritic dust provide important constraints on the formation of the Solar System and the early evolution on Earth.

Laboratory experiments on organic and refractory dust, as well as on various forms of ices, have made strong progress in the recent years. The production of materials is performed by different techniques and several methods are applied to investigate the morphology, the structure, the chemistry and the optical behaviour of the samples. The results obtained by various groups are often based on different experimental approaches and are, therefore, heterogeneous. Thus, it is important to compare different results for a correct interpretation of astronomical observations. On the other hand, it is clear that experimental techniques must be improved and must include new diagnostic tools and new approaches. In this sense, it is quite important to define some guidelines for future laboratory work by discussing already used and innovative techniques.

As far as the processing of cosmic material is concerned, a wide range of results is available in the literature. However, a homogeneous interpretation of data is hard, without a proper knowledge of the starting material characteristics and of the detailed experimental procedures applied. Also in this field the need of a careful correlation analysis among different results is evident in order to identify the experimental methods which appear promising for future research projects.

Of course, the most important step is to try to link the results obtained in laboratory to the observational data for two main aims: a) to verify to which extent laboratory simulations can be actually applied to interpret observations; b) to check whether evolutionary paths simulated in the laboratory are observed in space. This approach sheds light on several of the astrophysical open problems mentioned above. Last but not least, the formation paths which strongly link dust, ices, molecules and gas must be critically revised in order to define the compatibility between models, observations and experiments.

2. Objectives of the Workshop

Following the recommendations issued during the meeting of the ISSI core team on “The role of laboratory experiments in the characterisation of cosmic material”, held in Bern on 6-8.10.1999, some main items to be discussed during the Workshop to be held on 8 – 12 May 2000 have been identified.

<u>2.1 Laboratory experiments: approach</u>

The main aspects that drive the characterisation of cosmic dust and ice analogues in laboratory are:

Aspect	**Materials**		
	Silicates and other Oxides	**Carbon**	**Ices**
Production	• from gas phase • natural materials		
	• sol-gel reaction • melting • grinding	• from ices • from solids	• condensation • surface reactions • cluster beams
Processing	• thermal • ion, UV, X-ray, shocks		
	• H atoms		• H, C, N, O atoms
Assessment of characterisation methods	• FUV-FIR spectroscopy • TEM, SEM • EDX • Raman • mass spectrometry • PIXE • neutron spectroscopy • photoluminescence • AFM		
		• depletion spectroscopy	• LC • GC • HPCL
Parameters	• temperature (low to high) • doses • size • porosity		
		• C/H • hetero-atoms • hybridisation ratio	
Relevance of techniques for samples returned from space			

The following considerations must be accounted for:

- *It is important to distinguish between production techniques and processing that try to "simulate" the astrophysical conditions from those that are limited to "simulate" materials whose properties mimic those observed in space.*
- *The selection of laboratory materials as candidate to simulate cosmic dust must be based on a complete test of the spectral properties as well as on formation, evolution and elemental constraint considerations. Moreover, chemical matches allowed by meteorites and IDP’s must*

confine the range of likely products. By this approach it is possible to identify most relevant materials.

- *It is important to ascertain the degrees to which different possible formation mechanisms play a role in producing interstellar, cometary, and meteoritic materials. In so doing we understand better under which circumstances these various materials are formed (i.e. in the gas or on surfaces, for ice and refractories, or biotically).*
- *Since remote sensing is all we can hope for in most cases, spectral details are the most important probes. By combining information from different techniques it will be possible in differentiating between different material physical and chemical characteristics.*
- *When comet sample returns will become a reality, it will be possible to judge the relative importance of different interstellar/solar nebula processes (i.e., cosmic ray bombardment, UV photolysis, thermal processing etc.) that went into making up the primeval material that formed the Solar Nebula. It will be very important to exploit as many techniques as possible simultaneously, and further see if specific characteristics can be associated with spectral nuances. The techniques for the analysis of samples returned from space must be developed in contact with other scientific communities (e.g., glaciologysts). To this end actions towards relevant institutions (ESA, NASA) must be promoted.*
- *It is important to characterise the minor ice components and probe the surface versus bulk reactions of incoming radicals and atoms with the ice. It is important to truly understand the chemistry induced by energetic processing and to identify distinguishing characteristics of particle bombardment vs. photon processing vs. thermal processing. This is particularly important in unrevealing cometary processes for sample return missions. Lastly, a key challenge is to understand the interplay between ice surface/bulk chemistry and gas-phase chemistry.*

2.2 Laboratory experiments: problems

Key open problems in different areas of laboratory investigation are:

General problems	• Isotope effects • Size effects: single grains vs. clusters, spectral behaviour • Optical constants: comparison
Problems in sample production	• PAH's from organics et al. • Organic mantles • Silicates: chaotic vs. crystalline • Molecules on grain surface: methanol, CO_2, ... • Determination of stable nucleation structures
Problems in processing	• UV photon effects: two photon effects, ... • Shocks on grain mantles • Sputtering, chemi-sputtering • Time scale in laboratory vs. space • Chemical processing by UV, ions, X-rays, ... • Formation paths of crystalline silicates
Problems of characterisation	• Isolated grains and matrix effects • Gas phase spectroscopy of PAH's • Spectroscopy and luminescence of neutral and ionised PAH's, clusters, closed shell aromatic species
Problems with ices	• Detection of free radicals • Surface and bulk chemistry induced by ion/radical accretion vs. energetic processes

The following warnings have been issued:

- *A large fraction of extraterrestrial dust is made of both carbonaceous and silicate materials. It is not yet clear if such a mixture is the result of aggregation of pure carbons and pure silicates or if the mixing already occurs at the microscopic level. Efforts should be done in the laboratory to produce particles containing Si, O, and C at the same time.*
- *A relevant question is to establish when laboratory spectra can be directly comparable with observations without the need to consider shape/size effects.*
- *Production of key ice species, such as methanol and carbon dioxide, on grain surfaces has to explain why carbon dioxide is more or less constant (with respect to water) in environments with very different physical conditions, while methanol seems to be formed only at high-T ($\leq$ 100 K) regions around massive stars. Is this related to some catalytic process of grain surfaces?*
- *Caution must be applied in UV irradiation experiments when UV flux is much higher than in space. The lifetime of UV produced radicals (at low T, in particular) must be addressed.*

2.3 Astrophysical problems and laboratory role

Here following is a list of key questions that deserve further investigation about the formation of materials in space:

1. Origin of PAH's and C-particles: which comes first ?
2. Crystalline silicates in comets and disks
3. Size distribution
4. Formation and processing of materials and mantles in space
5. Where are sulphur, Si, iron ?

Here following is a list of spectral features that still need observations and laboratory experiments for definite identification:

1. UV bump and FUV rise in extinction and the 3.4 μm band: search for correlation
2. The 3.4 μm band vs. environment (e.g.: post AGB stars, IS)
3. The FUV extinction rise: absorption or scattering ? PAH's vs. nano-particles vs. grains ?
4. The 21 μm in post-AGB stars and the 26 – 30 μm features
5. Interpretation of other "exotic" mid-IR spectra of CSM, ISM (ISO data)
6. ERE
7. DIB's vs. UIB's (limited agreement with PAH's)
8. Si-H non identification

3. Organisation of activities during the workshop – Notes to participants

- The workshop is organised in plenary sessions and splinter meetings of three working groups
- The WG's are organised on the following main subjects:
  - silicon based materials
  - carbon based materials
  - ices
- During the plenary sessions there will be a few overview presentations (about 30 min., including discussion)
- During the WG splinter meetings short presentation (5-10 min.) from other participants are expected
- **All participants are invited to present their contributions during the splinter meetings. They are requested to <u>send to me by March 15 a title and a short abstract of their presentation</u>**
- The rest of time is dedicated to open discussion
- The topics to be covered during the sessions of the WG's are (see section 2):
  1. main aspects of laboratory experiments to characterise cosmic materials: production, processing, assessment of characterisation methods and key parameters (section 2.1)
  2. problems connected to laboratory experiments (section 2.2)
  3. unsolved astrophysical problems that can benefit from the use of laboratory data: indication of future perspectives (section 2.3)
- During the WG's sessions the topics mentioned above will be discussed. A summary of the results of the splinter meetings will be prepared in written form during the WG's sessions and presented during the plenary sessions
- **It is expected that at the end of the workshop one or more documents will be agreed and closed, where the results of discussion(s) are reported**
- **It is important that participants contribute to the preparation of the documents with their own material, such as figures, data, short reports. So you are invited to come well equipped with material in paper or, better, electronic formats for easier use and assembly**
- **The final goal is to prepare a general summary that is agreed by the whole group of participants and various other documents on the "hot" subjects that will be discussed during the workshop**
- **At the end of the meeting it can be decided that part or all the produced and assembled material will become matter for common publication(s) of part or all the team. This would represent "the" real success of the workshop (as also stressed by ISSI) !**

4. Participants and (suggested) composition of working groups (WG's)

SILICON-BASED MATERIALS
J.R. Brucato, <u>L. Colangeli</u>, L. D'Hendecourt, <u>Th. Henning</u>, F. Huisken, C. Jaeger, E.K. Jessberger, V. Pirronello, T. Stephan, L.B.F.M. Waters
CARBON-BASED MATERIALS
L. Allamandola, G. Baratta, P. Brechignac, M. Greenberg, O. Guillois, D. Hudgin, C. Joblin, <u>V. Mennella</u>, H. Mutschke, <u>C. Reynaud</u>, F. Salama, S. Wada
ICES
M. Bernstein, <u>P. Ehrenfreund</u>, A. Kouchi, M.H. Moore, M.E. Palumbo, St. Schlemmer, W. Schutte, <u>G. Strazzulla</u>, A.G.G.M. Tielens, N. Watanabe

Chairmen of WG's are underlined

5. PROGRAM (preliminary)

8 May 2000		
9.00 – 9.20	Welcome	V. Manno – J. Geiss
9.20 – 9.40	Objectives of the workshop	L. Colangeli – Th. Henning
9.40 – 10.00	Working group formation	
10.00 – 10.30	Coffee break	
10.30 – 11.00	How to make amorphous ice in laboratory	A. Kouchi
11.00 – 13.00	Splinter WG's on: "Laboratory experiments – approach and problems" Short presentations by WG members + open discussion	
13.00 – 14.30	Launch break	
14.30 – 15.00	Experiments on carbon-based macro-molecules	C. Joblin
15.00 – 16.00	Coffee break	
16.00 – 18.00	Splinter WG's on: "Laboratory experiments – approach and problems" Short presentations by WG members + open discussion	

9 May 2000		
9.00 – 9.30	Experiments on silicates	J.R. Brucato
9.30 – 10.30	Splinter WG's on: "Laboratory experiments – approach and problems" Open discussion	
10.30 – 11.00	Coffee break	
11.00 – 13.00	Splinter WG's on: "Laboratory experiments – approach and problems" Preparation of report	
13.00 – 14.30	Launch break	
14.30 – 15.00	Experiments on carbons	H. Mutschke
15.00 – 15.20	Working group 1 report	
15.20 – 15.40	Working group 2 report	
15.40 – 16.00	Working group 3 report	
16.00 – 16.30	Coffee break	
16.30 – 18.00	Open discussion and resolutions	

10 May 2000		
9.00 – 9.30	Observational evidences on carbon properties	A.G.G.M. Tielens (TBC)
9.30 – 10.30	Splinter WG's on: "Astrophysical problems and laboratory role" Short presentations by WG members + open discussion	
10.30 – 11.00	Coffee break	
11.00 – 13.00	Splinter WG's on: "Astrophysical problems and laboratory role" Open discussion	
13.00 – 14.30	Launch break	
14.30 – 15.00	Observational evidences on silicate properties	L.B.F.M. Waters
15.00 – 16.00	Splinter WG's on: "Astrophysical problems and laboratory role" Open discussion	
16.00 – 16.30	Coffee break	
16.30 – 18.00	Splinter WG's on: "Astrophysical problems and laboratory role" Preparation of report	

11 May 2000		
9.00 – 9.30	Observational evidences on ice properties	P. Ehrenfreund
9.30 – 9.50	Working group 1 report	
9.50 – 10.10	Working group 2 report	
10.10 – 10.30	Working group 3 report	
10.30 – 11.00	Coffee break	
11.00 – 13.00	Open discussion and resolutions	
13.00 – 14.30	Launch break	
14.30 – 16.00	Splinter WG's: Preparation of documents	
16.00 – 16.30	Coffee break	
16.30 – 18.00	Splinter WG's: Preparation of documents	

12 May 2000		
9.00 – 9.30	Splinter WG's: Preparation of documents	
9.30 – 10.00	Splinter WG's: Preparation of documents	
10.00 – 10.30	Summary	
10.30 – 11.00	Coffee break	
11.00 – 13.00	Summary and conclusions	

6. Participation, hotel booking and accommodation

For your hotel booking, please contact:
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Please, send also to me and to Mrs. Indermuehle the exact indication of your arrival and departure dates and time.

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