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R O U N D - T A B L E   D I S C U S S I O N

Second International Workshop on Amorphous and Nanostructured Chalcogenides (Sinaia, Romania, 20-24 June, 2005)

Chairmen: Guy Adriaenssens, Paul Allen, David Strand
Friday June 24, 2006, 9:30 -12:30, Hotel Sinaia

D. Strand (ECD, USA):
- For phase change applications faster and faster switching is needed
- More materials must be studied
- A challenge: how the problems could be approached ?

D. Tsendin (Joffe Physico-Technical Institute, Sankt-Petersburg, Russia):
- High Tc superconductivity in chalcogenides must be demonstrated experimentally
- The doping of chalcogenides depends on the purity in the stressed-rigid state
- In the future new structures will be designed by using the computer power, as in the case of drug design.

M. Poulain (Rennes University, France):
- (to Strand) what is the relation of the switching with the polarization of the \laser beam ?

G. Adriaenssens (University of Leuven, Belgium):
- (to Strand) how the layers in chalcogenide phase change memories orient themselves by switching the beam polarization ?

D. Strand (ECD, USA):
- the photo-transformations seems to be not large in nanometric structures; very small pieces of chalcogenides must be studied (100 nm in diameter on Si wafer)

V. Mitsa (Uzhgorod University, Ukraine):
- a- As-S system must be studied. The realgar type configuration exists or not ?
  The position of the absorption edge must be carefully checked in the system:
  $As_4S_4 – As_2S_3$.
- the transition layer between substrate and chalcogenide film is important. It seems that the thickness of this layer is 30 nm, much higher than in other cases.
  Why ?
- Films on silicon are good for reflectors and modulators

P. Allen (Richland, Pacific Naval Lab., USA):
- Doing glass
- characterizing glass
- my group creates components (builds and investigates)
- this is a good occasion to learn what every partner makes and how is possible to cooperate in the frame of NACNOG Consortium

M. Fekeshgazi (Inst. Semicond. Physics, Kiev, Ukraine):
- the chalcogenides open interesting problems in optics (small chalcogenide clusters in various oxide matrices are important as modulators for lasers/laser with Q-modulation)
- interdiffusion between layers are important for multilayer stacks
- the modulator must be calculated; it must work in the optical filter
- the chalcogenide struvcture for holography is interesting; now polymers are used with success.

D. Tsendin (Joffe Physico-Technical Inst., Sankt-Petersburg, Russia):
- the photo-structural changes are produced for not too intense illumination as that needed for photo-crystallization; the light can recover the initial structure, and this is carried out through an intermediary state.

M. Poulain (Rennes Univ., France): (answer)
- The crystallization occurs for enough vibration energy to trigger the change.

S. R. Elliott (Cambridge Univ., UK):
- the glasses for phase-change memories are at the limit of stability (the case of telluride glasses)

G. Adriaenssens (Leuven Univ., Belgium):
- main part of the research in chalcogenides is carried out in the academic institutions; many esoteric problems are discussed and they are, later, taken and introduced in technology. The engineers have a different education, but they can help substantially the research.

P. Allen (Richland, Pacific Naval Lab., USA):
- Government laboratories **and not industry** make applications !

S. R. Elliott (Cambridge Univ., UK) :
- it is of great help to discuss the not yet resolved problems

P. Haussler (Chemnitz Technical Univ., Germany):
- It is important how to work together !

M. Wuttig (Inst. of Physics, Aachen, Germany):
- we must to be more optimistic; the science-man helps the technologist, which put the scientific problems !
- young persons must join in order to solve the interesting scientific problems

G. Adriaenssens (Leuven University, Belgium):
- the interface between industry and science must exist (or must be formed); an example is X-ray imaging, where the industry helped very much; the hospitals were also interested

M. Wuttig (Inst. of Physics, Aachen, Germany):
-In Aachen these problems will be posed in the future 5 years !

D. Strand (ECD, USA):
- The viewpoint of Guy is important. The money is important. Stan (Ovshinsky) asked for researches in phase change memories to professors that applied for grants !
-in the universities the number of publications is important. Nevertheless, they must retain from publishing when patents are in view.
- in the work with academic institutions the time scale is larger than that occurring when industry is involved.

M. Wuttig (Inst. of Physics, Aachen, Germany):
-The industry will allocate money for longer studies (3 years); nevertheless, there are not many investors in science

V. Mitsa (Univ. Uzhgorod, Ukraine):
-synthetizing of bulk glasses for optical devices, recording media
- every year 100 students enter into the dept. of solid state physics
- preparation of interference filters with transition layers
- preparation of standard filters for infrared light (for industry)
- chalcogenide for temperature measurement

- partnership with USA for material processing

S. R. Elliott (Cambridge Univ., UK):

- There are problems not resolved for 20 years; now we have computers and femtosecond lasers to approach these problems with success.
What we don't know ?

1. Structure
- the presence of quasi-molecular fragments
- the nature of medium-range ordering
  exent of the planarity in As-Ch
  correlation range for $AsCh_3$ pyramidal correlations
  correlation range for $GeCh_4$ tetrahedral correlations
  ordering of interstitial voids in non-tetrahedral materials (?)
- Does Boolchand intermediate stress-free state exist ?

2. Defects

- nature of diamagnetic (coordination) defects C_3^+, C_1^-, As_4^+, As_4^-
- nature of paramagnetic coordination) defects C_3^o, C_1^o, As_4^o
- Ge_2 (as in SiO_2) ? What is the relation with oxides ?
- Homopolar bonds ↔ "long" bonds ?
- Impurities

3. Vibrations

- origin of the boson peak ?
- origin of far-IR (THz) optical absorption ?
- how to detect localized states – e.g. at upper optic band edge, upper Raman?

4. Photo-induced effects

- origin of metastable scalar effects (e.g. photodarkening, photo-bleaching, e.g. in As_xS_{1-x})
- origin of metastable vectoral effects (e.g. dichroism, birefringence)
- origin of dynamic effects (e.g. photo-fluidity)

5. Electronic structure

- origin of the Urbach edge (exponential tails)
- are band-tail states localized (if no defects) ?

- is midgap absorption defect-related ?
- are non-linear effects (e.g. two phonon absorption) related to deep defects, or polarizability ?
- how to increase the non-linear effects (e.g. $\chi^{(3)}$) → nanostructure

6. Electrical properties

- origin of switching effect ?
- origin of high ionic conductivity ?
- importance of polaronic effects in conduction ?
- existence of superconductivity at high pressure (Meissner effect) ?

7. Experimental

- samples, say with the same composition and density but prepared from different T_f and with different cooling rate (this will imply different amount of defects and/or different quality of the defects…)
- relation of amorphous chalcogenide to the liquid ones

8. Computer simulation

- how to simulate (optically) electronically states (e.g. for photodarkening) ? This needs proper description of excited states (e.g. K-S ground state) + validity of the adiabatic approximation (polaronic effects) ?
- problem of time-scale (e.g. < 1 ns); extend using coarse graining or Monte-Carlo approximation ?

Regarding the medium range order in chalcogenides: are there quasi-molecular fragments or broken molecules ? During quenching from different temperatures it is possible to see if the density is preserved, and which is the true structure ? Do exist planar structures ? How extended are these structures ? Which is the MRO correlation range in chalcogenides? But in amorphous Ge or Si ? How the atoms, in fact, the voids are packed ? The Boolchand phase really exists ? If yes, how this phase is structured ?

Regarding the defects: are there under and over-coordinated defects ? How dirty are the materials ? The impurities dominate the electronic properties. We must control the structure. The solutions will be given by experiments.

Regarding vibrations: low frequency vibrations are important. The infrared absorption is important. The physical basis of the problem is not yet known. How the band edge vibrations can be seen in experiment? It is a very difficult problem!

Regarding metastability of the chalcogenides:
What is the origin of the photo-induced effects? How they depend on polarization? The orientation can be switched. What is the origin of this effect ?

Regarding the optical aborption: why the absorption tails are localized ? Which is the origin of the tails ? The cause could be the impurities at very low level. Are these related to the non-linear optical effects ? If yes, why ? How to relate the effect of polarizability to defects ? It seems that the polymorphism is important, especially in nanostructures.

Which is the electronic structure of the conducting phase, before crystallization ? Why the chalcogenides could be applied in ionic conduction domain? The material is very flexible. How could be related the electronic coupling phenomenon to conductivity ? Which is the nature of superconductivity ? We must learn much before making superconductivity models !

Regarding computer simulation: the description of the electronic excited states is important; ground state and excited state are completely different.

P. Haussler (Chemnitz Technical Univ., Germany):
- the structure is not independent of the electronic structure
- the collective effects are important
- independent electrons does not exist
- if structure changes then the electron dynamics changes; the systems are coupled.

D. Tsendin (Joffe Physico-Technical Inst. Sankt-Petersburg, Russia):
- the defects in chalcogenides are important
- Jahn-Teller effects do exist
- pairing in chalcogenide localized effects
- if pairing is absent, then the final state must be analyzed

M. Wuttig (Inst. of Physics, Aachen, Germany):
- the relation between the structure with short range and long range memories must be investigated
- anorganic and organic materials must be compared relative to the ordering

S. Dalgyc (University of Trakya, Edirne, Turkey):

- the glass forming is an interesting field of research
- for understanding the phenomenon the interaction potentials are important
- the potentials are also important for network dynamics
- the potentials are useful for mechanical properties, for quantum calculations, for multiple well investigation and understanding.