



# VUV SPECTROSCOPY BEAMLINE

## Proposal for the Central European Synchrotron Laboratory

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### Introduction

Ellipsometry and spectrophotometry are basic methods for the study of material optical properties. Basically, it means the determination of the dielectric function of the material but other parameters such as roughness, thin film thickness and the presence of transitional layer or native overlayer can be assessed too. The combination of ellipsometry and spectrophotometry is seldom used because the users are convinced that these two methods provide the same information. However, this is true only in the case of optically ideal systems whereas for characterization of the non-ideal systems the complete information about the light in far field, i.e. all four components of the Stokes vector, is required. Examples of such cases, in which the combination of ellipsometry and spectrophotometry is advantageous, are surface roughness, inhomogeneity or lateral non-uniformity. It should be emphasized that, as far as we know, the VUV ellipsometry at the synchrotron beamline is available only in one facility in the world, BESSY II.

The spectral range of the proposed VUV synchrotron beamline (5–40 eV) ideally complements the existing commercial UV–VIS–NIR ellipsometers and spectrophotometers available for instance at the Department of Physical Electronics (DPE) at the Faculty of Science, Masaryk University in Brno (ellipsometer and spectrophotometer spectral ranges are 0.6–6.5 eV and 0.05–6.5 eV, respectively). The proposed beamline allows studying the optical properties of solids beyond the spectral range of the commercial devices and, furthermore, the overlap of its spectral range with the table-top instruments allows corrections of systematic errors inherently present in the spectroscopic measurements carried out in the restricted set-ups of the UHV apparatuses.

Additionally to the material optical properties and information about sample defects, the information about the band structure of the studied materials can be obtained with a proper parametrization of the dielectric function or directly the density of states. It can be particularly important for the basic research of novel materials and for the development of new dispersion formulae. Since the energies of interband transitions range from visible/UV to VUV it is important to extend the table-top optical measurements to the VUV synchrotron region. Recently, we proposed the dispersion models based on the parametrization of density of states (PDOS) and parametrization of the joint density of states (PJDOS) that can be applied to many different disordered solids [1]. Although the PDOS and PJDOS models reached excellent agreement with the optical measurement in the visible/UV range the omission of the high excitation states was a certain weakness from the theoretical point of view. It can be eliminated by adding more conductive bands corresponding to higher excitations but the confir-

mation of the models then needs optical measurements in the VUV region.

### Materials

VUV ellipsometry and spectrophotometry is required to study the band structure of a wide range of technologically interesting materials including crystalline, polycrystalline, amorphous as well as nanostructured and nanocomposite materials which investigation is of high priority in many research fields and EU Framework Programmes. These materials can be applied in microelectronics, Micro Electro Mechanical Systems (MEMS), optics, material engineering, biotechnologies, etc.

Hard carbon materials find many applications in tribology, MEMS and as protective coatings due to their unique properties such as high hardness, chemical inertness and biocompatibility. In case of microcrystalline and nanocrystalline diamond, diamond-like carbon (DLC) and their modifications (doping, nanocomposites) it is important to control the structure of these materials, namely the content of  $sp^2$  and  $sp^3$  bonded carbon. The relative content of  $sp^2$  and  $sp^3$  bonded carbon can be determined from the ratio of  $\pi$  and  $\sigma$  electrons. While the absorption peak corresponding to  $\pi$  electrons (responsible for the weak graphitic bonds) lies in the visible region, the absorption corresponding to  $\sigma$  electrons (responsible for the strong diamond bonds) lies in the VUV region, with the maximum of absorption at about 13 eV. Similarly, the absorption of materials for VUV optics, e.g. in VUV lithography required for Ultra Large Scale Integration (ULSI), such as  $MgF_2$  and  $LaF_3$ , starts above 10 eV. Moreover, the quality of their surfaces as concern roughness and uniformity has to be controlled and verified. It can be reliably done by the combination of ellipsometry and spectrophotometry. In the case of study of biomaterials, the transitions between the localized electronic states corresponding to the characteristic structures are observed. The energies of these transitions lie not only in the visible and near UV region, but also in the VUV region.

Materials crystallizing in perovskite structures exhibit wide range of interesting properties, for example materials with ferroelectric properties and structural phase transitions ( $SrTiO_3$ ,  $BaTiO_3$ ,  $PbTiO_3$ ), antiferroelectrics ( $PbTiO_3$ ), materials with special optical properties ( $KTaO_3$ ,  $KNbO_3$ ) and their mixtures (PZT, BST, KTN) or materials with both ferroelectric and magnetic properties, i.e. multiferroics ( $BiFeO_3$ ). These include use as dielectric materials in capacitors, as oxygen ion conductors in sensors, as substrates for high  $T_c$  superconductors, or as piezoelectric materials in actuators. A thorough understanding of most of these properties requires the knowledge of the electronic structure of the bulk material.

## Scientific case of the proposed beamline

We propose the installation of two spectroscopic techniques for the VUV beamline, i.e. ellipsometry and spectrophotometry, at the Central European Synchrotron Laboratory (CESLAB). The proposal is justified by a uniqueness of their combination at the synchrotrons in world. This combination is required for the study of non-ideal samples. It can be either realized by two separate UHV chambers or, preferentially, in the one chamber set-up.

## Beamline

The beamline will operate with horizontally polarized beam in the energy range from 5 to 40 eV with resolution  $> 25\ 000$ . The appropriate insertion device will be specified later.

## Inspiration in the world

The design of proposed beamline is motivated by the following beamlines in the world:

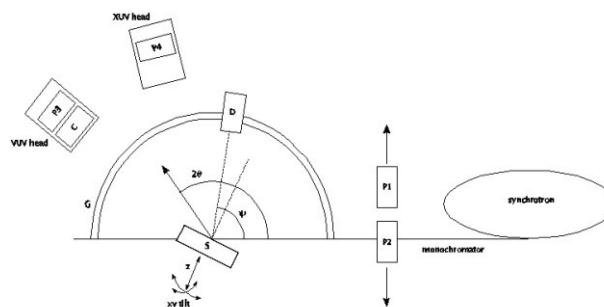
- BESSY II: Beamline “3m-NIM-A” for spectroscopic ellipsometry in the range 2–40 eV.
- BESSY II: Beamline “Optics Beamline” for variable angle spectroscopic reflectometry in the range 20–1300 eV.
- UVSOR: beamline “BL7B”.

## Optics hutch proposal

The hutch will be specified after the experimental hutch requirements are known in more details.

## Experimental hutch proposal

Due to the uniqueness of the proposed experimental device it is not possible, at this stage, to provide detailed technical specifications. One of the possible set-ups combines the ellipsometry and spectrophotometry in one VUV chamber (see fig. 1). The light beam from the synchrotron falls on the sample through the changer of polarisers switching between polarisers P1, P2 and no polariser. The P1 is  $\text{MgF}_2$  prism polariser that can be used for the VUV region 5–10 eV. In the XUV region 10–40 eV, a triple reflection gold mirror type polariser P2 must be used instead. The vertically mounted goniometer G of the spectrophotometer moves with the arm of the detector D in the range of  $\theta = 0\text{--}180^\circ$ . The sample stage performs the following motions: rotation around the same axis as the detector goniometer  $\phi = 0\text{--}90^\circ$ , fine z-positioning and fine adjustment of the surface plane tilt in two perpendicular directions. The sample has to be able to move out of the light path when the detector D is at  $180^\circ$ , in order to measure the incident light intensity for the determination of sample reflectance. Two ellipsometer heads, i.e. VUV and XUV, are mounted in fixed positions at cca  $70^\circ$  and  $55^\circ$ . The VUV head can be separated from the VUV chamber with an  $\text{MgF}_2$  window and nitrogen purged. We propose to base the VUV ellipsometer head on the principle of phase-modulation, i.e. consisting of the photo-elastic compensator C, polariser P3 and detector. The XUV ellipsometer head will consist of a second rotating triple reflection gold mirror polariser P4



and detector, i.e. rotating analyser ellipsometry will be used.

## Sample environments

Preferentially, the measurement UHV chamber should be equipped with a load lock and an HV sample preparation chamber which can be used for cleaning the samples prior to the optical measurement by thermal annealing or modification of the sample surface by plasma or ion beam. The sample stage in the UHV measurement chamber should be optionally equipped with liquid nitrogen cooling or He cryostat for low temperature measurements or with a furnace allowing to measure at high temperatures.

## User community

User community for this beamline covers users from academia and research institutions, universities or industry growing, preparing hard and soft condensed matter samples (solid state physics, superconductivity, thin films and coatings), as well as analytical laboratories, including the Czech community “Nanoscience for society”.

## Academic Czech user community

The Czech user community working in ellipsometry and spectrophotometry:

1. Masaryk University, Brno. Group of D. Franta, D. Nečas, L. Zajíčková, I. Ohlídal
2. Institute of Physics, Prague. Group of D. Chvostová, A. Deyneka, V. Železný
3. University of Pardubice, Pardubice. Group of J. Mistrík
4. Technical university, Brno. Group of V. Čech.
5. University of Ostrava, Ostrava. Group of K. Postava
6. Producers of samples and nanostructures, including industry and private companies.

## Central European community

The potential user community covers users from Slovakia (e.g. Institute of Physics, Bratislava) and from Austria (universities in Wien and Linz).

## References

1. Daniel Franta, David Nečas, Lenka Zajíčková, Models of dielectric response in disordered solids, *Optics Express* **15** (2007) 16230–16244.