Beamline 7: Vacuum ultraviolet spectroscopy

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Potential Research Fields

Life sciences

- Biological research and drug design
- Plants and crops

Physical sciences

- Advanced materials
  - Nanomaterials and composites
  - Metals and alloys
  - Micro-electronic and magnetic materials
  - Biomaterials
- Chemical reactions and catalysts

Introduction

A high resolution beamline for a range of vacuum ultraviolet (VUV) spectroscopic studies of solids, atoms and molecules – covering photon energies from 10 eV to 350 eV – holds particular promise as a generator of significant new fundamental science, and strategic work of future technological importance. A particular strength of the proposed beamline is the potential to bring several powerful surface science techniques to bear on a particular problem under the same conditions.

Advantages of a Synchrotron Source

A synchrotron radiation source is essential for the proposed VUV experimental techniques because they use all the features of synchrotron light, namely the tunability, the circular and linear polarisation, the coherence and the single- and multi-bunch timing modes. These combined features enable the coincidence detection of physical and chemical reaction particles and their time development. The proposed studies are not possible without a synchrotron.

User Community

The number of users with existing synchrotron experience in the VUV area in Australia is significant (at least eight groups) but not large in comparison with other synchrotron techniques. Access to VUV beamlines has not been available through the ASRP to this time. The groups are, however, distinguished by their extensive experience and an advanced capability in terms of both synchrotron and end-station instrumentation.

Due to the ultra high vacuum nature of VUV beamlines, and the essential requirement to prepare atomically clean single crystal samples in situ, a typical beamline visit is of 2–3 weeks duration for solid state experiments. For gas phase experimentation, custom built end stations are commonly required with possible consequences in terms of time lost changing instrumentation. Experiments involving coincidence techniques are particularly time intensive.

Using Germany's BESSY facility as a model, eight user groups can be offered two 2-week periods per year. On this model, an Australian VUV beamline would already be over subscribed.

Research Applications

Existing synchrotron facilities dedicated to the VUV region include comparable beamlines in operation at BESSY (Berlin), Elettra (Trieste) and ALS (Berkeley). A wide range of spectroscopic and microscopic techniques is in evidence at these facilities, with several of them having unique Australian components that have made them world leaders. These features, and new developments, will be established in the VUV beamline of the Australian Synchrotron.

Angle resolved photoemission spectroscopy

Angle resolved photoemission spectroscopy is the pre-eminent technique for the elucidation of the electronic structure of crystalline solids.

Solid state studies

Although the photoemission technique has many applications at higher energies, it is in the VUV region of the spectrum that angle resolved data is essential for providing a sufficiently detailed view of the electronic band structure of crystalline solids.

By 2007, state of the art instrumentation will require energy resolution of a few meV coupled with angular resolution significantly better than 1 degree. Instrumentation will be required to resolve fine structure in many materials of technological value and to investigate electronic structure beyond the one-electron approximation.

The availability at synchrotron sources of circularly polarised radiation that can be rapidly switched between both helicities enables a suite of magnetic circular dichroism experiments to be undertaken. These can reveal spin-orbit interactions in the conduction band to derive the electronic structure of magnetic materials.

Applications include understanding the properties of shape memory alloys, of colossal-magneto-resistance alloys and of strongly correlated materials such as the cobaltates and high temperature superconductors.

Photoemission from the valence band is very attractive for studying chemisorption on semiconductor surfaces.

The study of low binding energy core lines of vacuum fractured, conducting (or small band gap) mineral single crystals, in conjunction with detailed valence band studies can illuminate interrelationships between crystal and electronic structure, bulk vs surface states and, in the end, the reactivity of such materials.

Novel inner shell Auger photoemission coincidence spectroscopy (APECS) has a unique ability to disentangle signals originating from different sites within a solid and/or from overlapping spectral features, such as surface alloys in metallic systems that intermix only in the first layer and then can influence the underlying electronic structure. APECS shows an enhanced surface sensitivity compared to non-coincidence photoemission.

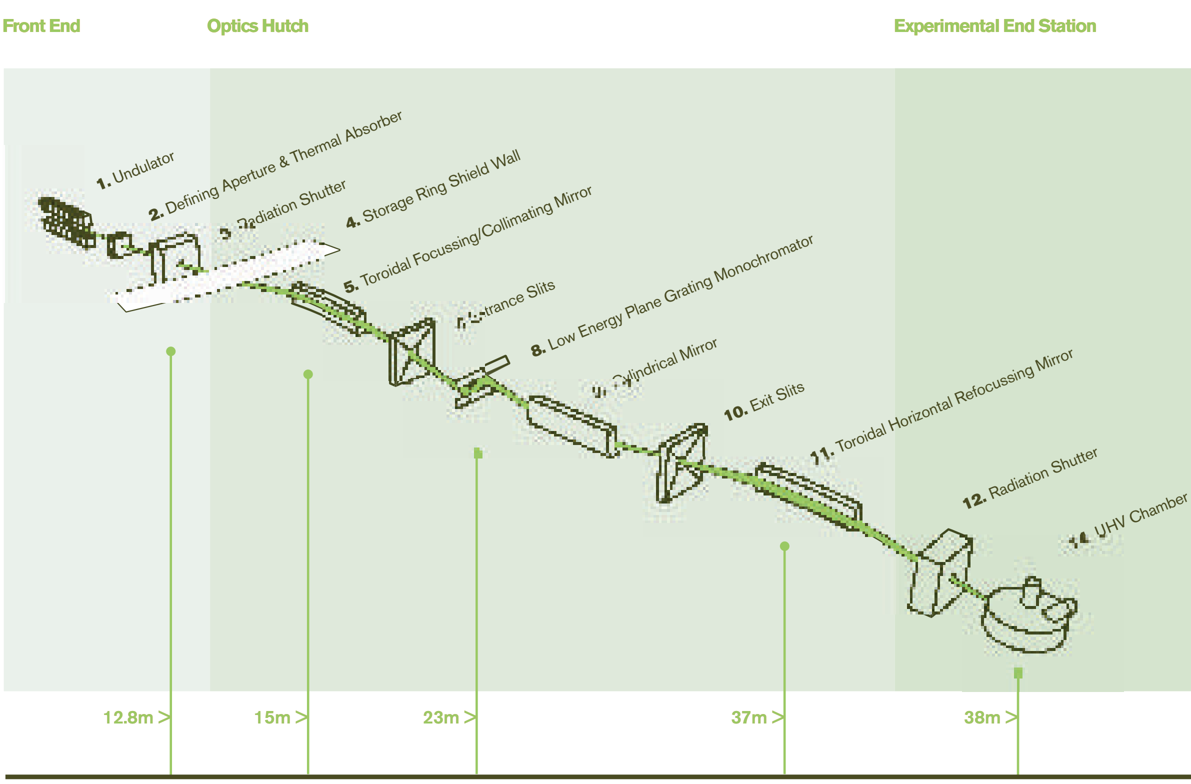
Gas phase studies

Angle resolved photoemission measurements have traditionally been used to validate molecular orbital calculations of both stable and transient molecules. Synchrotron VUV gas phase studies allow investigation of electron correlations in bound and continuum states, electron exchange and spin-orbit effects, interference and coherence, orbital and magnetic dichroism effects and relativistic effects.

New techniques, such as angle-resolved photo-electron-photo-ion coincidence spectroscopy now make possible, for the first time, the study of electron-ion momentum vector correlations and reveal intermolecular scattering and associated interference. Exploration of the dynamics of the photo-excitation of free molecules and the high resolution VUV spectroscopy of atmospheric molecules are examples of topics of strong current interest.

Double photo-ionisation, studied using coincidence angular distribution techniques, may be used to investigate the important question of coherence in atomic physics.

A recently developed technique with great promise involves the investigation of the intrinsic width of selected atomic states via fluorescent, rather than photo-ion emission. This technique also has particular merit for the optimisation and the determination of the resolution of VUV beamlines.



BEAMLINE 7 Vacuum UV Spectroscopy

Figure BL7.1. *Schematic of the VUV beamline*

Pulsed multi-bunched operating modes of the synchrotron enable an extensive list of time-of-flight spectroscopies, including rotational-vibrational, fragmentation modes and lifetimes of molecules as well as inner-shell effects.

Adsorbate studies

Synchrotron-based angle resolved VUV photoemission will enable studies on the identity and bonding of the successive surface-intermediates in various chemical vapour deposition (CVD) processes; the bonding of amino acids with metal surfaces; and the characterisation of carbon nanotubes, gallium nitride nanowires and silicon quantum-wire arrays.

Biosystems

Surface science has recently been increasing in prominence in the biomedical area, based on the fact that many biological reactions occur at surfaces. Thus any fundamental understanding of the biocompatibility of a medical device must take into account the properties of proteins and cells at interfaces, and the characteristics of local biological reactions. Principles worked out in surface science laboratories are likely to become the basis for ways of improving the function and durability of materials featured in a wide range of medical products.

The electronic properties and interactions of matter at an atomic level in biological environments are largely unknown. Yet the detailed understanding of these systems is crucial to the successful development of many new technologies that have direct impact in our community. Applications include medical implants, delivery systems (for example of radiopharmaceuticals), bio-sensors and chips for diagnostics, biomimetic materials (such as the construction of artificial skin or organs), and novel artificial photosynthetic devices.

VUV light is able to probe the valence and low-lying core states of many elements in the periodic table. The interaction of such states ultimately controls the complex interactions and properties observed in biological systems. The high flux and small spot size produced by the VUV beamline will allow for many ground-breaking experiments and studies to be performed on biosystems from a sub-Angstrom to micron scale.

As most biosystems are made of several functioning parts, small spot microscopy on objects as tiny as only a few nanometres to as large as several microns in size would be of tremendous importance in order to determine accurately the electronic state of each part.

Studies will initially focus on more traditional (but still as yet not understood) systems such as the electronic properties and structure of amino acids (essential building blocks) on various surfaces. Techniques such as high-energy resolution valence band and core level mapping as well as 'photon-in/photon-out' and 'photon-in/electron-out' scattering techniques will be used. One significant new direction would be the study of liquid–solid interfaces and multi-layered systems.

Beamline Design

The beamline would be matched to a long-period variable-polarisation elliptical undulator as source. A design study is currently being prepared by staff at the BESSY synchrotron facility in Berlin. It is expected that this undulator will deliver both linearly polarised and circularly polarised radiation and that the plane of linear polarisation can be rotated through 90 degrees from horizontal to vertical. Such capabilities are considered particularly important as they open up many possibilities relating to magnetic effects in solids and chirality effects in the gas phase.

The optical components of the proposed plane grating monochromator (PGM) beamline operate in glancing incidence reflection mode. All sections of the beamline must be maintained under UHV conditions ($<10^{-10}$ torr), in common with the end stations. A full description of the optical design is available[1], but for present purposes it is sufficient to point out that the final mirror causes the beam to be focussed to a spot of approximately 220 microns (horizontal) by 10 microns (vertical) at a position 1 metre behind the final mirror. The photon resolving power will be greater than 10,000.

Beamline 7 – Vacuum Ultraviolet (VUV)	
Source	Undulator (185 mm period), variably polarised
Energy range	10–350 eV
Resolution $\Delta E/E$	10^{-4}
Beam size at sample (horizontal × vertical)	220 × 10 micron
Special features	Ultra high vacuum (pressure $<10^{-10}$ torr)

1 R. Follath. A collimated PGM for the U125 operating at 3 GeV. Bessy report. Berlin 2003.