



Review

Understanding interface properties from high kinetic energy photoelectron spectroscopy and first principles theory

Sari Granroth^{a,d}, Weine Olovsson^b, Erik Holmström^c, Ronny Knut^d, Mihaela Gorgoi^e, Svante Svensson^d, Olof Karis^{d,*}

^a Department of Physics and Astronomy, University of Turku, FIN-20014 Turku, Finland

^b Department of Materials Science and Engineering, Kyoto University, Sakyo, Kyoto 606-8501, Japan

^c Instituto de Física, Universidad Austral de Chile, Valdivia, Chile

^d Department of Physics and Materials Science, Uppsala University, SE-751 21 Uppsala, Sweden

^e Helmholtz Zentrum Berlin, BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany

ARTICLE INFO

Article history:

Available online 24 August 2010

PACS:

79.60.Jv

71.20.Be

73.20.-r

Keywords:

High kinetic energy photoemission

Multilayers

Interface properties

Alloying

Electronic structure

Ab initio theory

ABSTRACT

Advances in instrumentation regarding 3rd generation synchrotron light sources and electron spectrometers has enabled the field of high kinetic energy photoelectron spectroscopy (HIKE) (also often denoted hard X-ray photoelectron spectroscopy (HX-PES or HAXPES)). Over the last years, the amount of investigations that relies on the HIKE method has increased dramatically and can arguably be said to have given a rebirth of the interest in photoelectron spectroscopy in many areas. It is in particular the much increased mean free path at higher kinetic energies in combination with the elemental selectivity of the core level spectroscopies in general that has led to this fact, as it makes it possible to investigate the electronic structure of materials with a substantially reduced surface sensitivity. In this review we demonstrate how HIKE can be used to investigate the interface properties in multilayer systems. Relative intensities of the core level photoelectron peaks and their chemical shifts derived from binding energy changes are found to give precise information on physico-chemical properties and quality of the buried layers. Interface roughening, including kinetic properties such as the rate of alloying, and temperature effects on the processes can be analyzed quantitatively. We will also provide an outline of the theoretical framework that is used to support the interpretation of data. We provide examples from our own investigations of multilayer systems which comprises both systems of more model character and a multilayer system very close to real applications in devices that are considered to be viable alternative to the present read head technology. The experimental data presented in this review is exclusively recorded at the BESSY-II synchrotron at the Helmholtz-Zentrum Berlin für Materialien und Energie. This HIKE facility is placed at the bending magnet beamline KMC-1, which makes it different from several other facilities which relies on undulators as the source. We will therefore also briefly describe some of the salient design features of this facility.

© 2010 Elsevier B.V. All rights reserved.

Contents

1. Introduction	81
2. The HIKE facility at the KMC-1 beamline	81
3. Interface properties in multilayer systems from HIKE and ab initio theory	82
3.1. First principles calculations of core-level shifts in an inherently disordered system	82
3.1.1. Computational methodology	83
3.1.2. Interface mixing	83
3.1.3. Simulation of spectra	83
3.1.4. First principles calculations of Ni/Cu multilayers	84

* Corresponding author at: Department of Physics and Astronomy, Uppsala University, Box 516, 75120 Uppsala, Sweden.

E-mail address: olof.karis@fysik.uu.se (O. Karis).

3.2. Interface properties in a model multilayer system: Ni/Cu multilayers.....	84
3.3. Alloying of Pt capped Fe/V multilayers.....	88
3.4. Towards applications: Interface properties in all-Heusler multilayers.....	89
4. Conclusions.....	91
Acknowledgments.....	92
References.....	92

1. Introduction

The inherent surface sensitivity of photoelectrons with kinetic energies in the range of 50–1000 eV is the explanation why the photoelectron spectroscopy has been key to many important contributions in the field of surface science (for example, see Ref. [1]). However, as the kinetic energy of the emitted photoelectron is increased the inelastic mean free path is also increased and can approach tens of nm for kinetic energies in the range of 4 keV and higher. Incidentally, the use of high energies to record photoelectron spectra is not at all new. In the very early days Prof. Kai Siegbahn and his co-workers were using Mo anodes as excitation sources where the $K\alpha_1$ and $K\alpha_2$ X-ray lines are found around 17.4 keV. Prof. Siegbahn's interest in photoelectron binding energies originated from his interest in nuclear spectroscopy and internal conversion, where part of the energy released in the decay of the nucleus is taken by a core electron that is emitted. To obtain the correct values for the nuclear transitions they thus required accurate values for the electron binding energies of the elements of interest [2,3]. The only detectors available to these pioneering electron spectroscopists were Gieger–Müller (G–M) counters that in many respects were a nuisance. Most importantly the window transmitted electrons only down to ~ 4 keV. It was hence impossible to realize anything else than electron spectroscopy with high kinetic energy electrons. Despite the obstacles, electron binding energies and even chemical shifts were determined with a surprising accuracy already in 1957–1958 [4–7].

The availability of new types of spectrometers with electrostatic lenses, new detectors and most importantly new narrow band excitations sources led to enormous advances in the field of electron spectroscopy during the 1960s. At this point the technique was already identified to have a huge impact on the investigation of surface electronic structure. In the early stages of exploiting synchrotron radiation as an excitation source for electron spectroscopies, Ingolf Lindau and Piero Pianetta pointed out the potential of using monochromatized hard X-rays from a synchrotron for photoelectron spectroscopy and also did some pioneering investigations at SLAC [8]. Despite this fact, there are not many reports of high energy photoemission until the beginning of the 21st century. Again this is simply a consequence of instrumentation advances. During almost three decades, photoelectron spectroscopy had matured into a very high resolution technique with a total resolution of some tens of meV or even better. With the availability of new bright synchrotron sources and monochromators with a resolving power in the range of 10^5 combined with electron energy analyzers capable of analyzing electron energies in the range of 10 keV with meV resolution, technology had finally reached the necessary level of perfection to fully enable the potential pointed out by Lindau et al. We refer the reader to one of the excellent reviews and facility reports that has been published over the last few years for a more complete picture of the wealth of activities ongoing within the field of high X-ray energy photoemission [9–18].

High Kinetic Energy photoelectron spectroscopy (HIKE) has lately attracted large interest and rapidly developed into a promising tool to address electronic properties of buried interfaces and

bulk layers [19–23,14,24–28], as it is one of the few methods that enable non-destructive bulk sensitive studies. At this point it could be pointed out that hard X-ray photoelectron spectroscopy (HX-PES or HAXPES) does not necessarily imply high kinetic energy of the emitted photoelectron (i.e., the HIKE range), as tender and hard X-rays provide access to much deeper core levels. The great advantage of HIKE is the accurate measurement of shifts in core-level binding energies of bulk atoms, which reflect changes in chemical environment and give us information about intermixing of interface atoms and alloying of the multilayers.

Multilayers have attracted interest in many fields because of their numerous practical applications and interesting properties. Nowadays, the development of technology is strongly correlating with the advance of nanodevices, built up by multilayers and thin films or superlattices. The thickness, composition and interface structure of the layers are used to tailor magnetic, mechanical and optical properties of the devices.

In this paper we review some of our work on analyzing interface properties in multilayer systems using high kinetic energy photoemission. We also describe the theoretical framework that is used to calculate and model experimental data. The paper is organized as follows. We begin by briefly describing the essential features of the HIKE facility at the KMC-1 beamline at BESSY-II in Berlin. The remainder of the paper is devoted to our multilayer studies. We first present our investigations on Cu/Ni multilayers, i.e., the system that we first investigated using our methodology. We have later revisited this system and we summarize our recent findings here. The following section is devoted to the description of the theory of calculating chemical shifts in alloys and disordered systems. We then finally present results from two systems, Fe/V multilayers and $\text{Co}_2\text{MnGe/Rh}_2\text{CuSn}$ multilayers, that have not been presented elsewhere to date.

2. The HIKE facility at the KMC-1 beamline

The HIKE experiments were carried out on the HIKE experimental station at the KMC-1 bending magnet beamline in BESSY, Berlin. The beamline is equipped with a high resolution double crystal monochromator which consists of three sets of crystals, Si(1 1 1), Si(3 1 1) and Si(4 2 2), that can be changed within some minutes. The resolution as a function of energy is given in Fig. 1. Despite the fact that the source is a dipole on the BESSY-II storage ring operating at 1.7 GeV, it is possible to obtain good working conditions in terms of resolution and flux between 1.7 and 12 keV, where there is of course always a trade-off between these quantities. As illustrated in Fig. 2, we note in particular that we have been able to record Ni core level spectra from Ni metal at 12 keV excitation energy. In Ref. [21] we used this possibility to show how differences in the screening of the core lead to differences in the satellite structure at the 1s and 2p levels respectively. In that study, the total experimental resolution was limited by the Si(4 2 2) crystals which is approximately 1.2 eV at 12.6 keV photon energy.

In order to achieve necessary working conditions for HIKE it is beneficial to design beamlines where concepts of soft X-ray beamlines regarding optical elements and beam paths to the experiment (windowless design up to end-station) are married to state-of-the-

Download English Version:

<https://daneshyari.com/en/article/5396376>

Download Persian Version:

<https://daneshyari.com/article/5396376>

[Daneshyari.com](https://daneshyari.com)