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ScienceDirect
Surface Science 600 (2006) 4464–4474
SURFACE SCIENCE
www.elsevier.com/locate/susc

Angle-resolved elastic-peak electron spectroscopy: Solid-state effects

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Received 10 April 2006; accepted for publication 3 July 2006
Available online 31 July 2006

Abstract

It has been frequently reported that characteristics of electrons elastically backscattered from solid surfaces (e.g., the angular distribution) are well described by Monte Carlo simulations of electron trajectories in solids. The theoretical model implemented in these simulations requires knowledge of accurate differential elastic-scattering cross sections (DCSs). In computational practice, the DCSs for isolated neutral atoms constituting the solid are used to simplify the calculations. In reality, the interaction potential between an electron and an atom inside a solid is different from the interaction between an electron and an isolated atom. In the present work, we study changes of the DCSs due to agglomeration of atoms. The interaction between an atom and an electron in the solid is approximated by the muffin-tin potential. It has been found that the DCSs are considerably influenced by the agglomeration of atoms for small scattering angles. The difference for silicon reaches 500% for silicon at 200 eV. On the other hand, electron elastic-backscattering probabilities calculated using DCSs from two potentials were only slightly affected. Calculations and measurements of elastically backscattered intensity were compared for 10 elemental solids, a number of emission angles from 35° to 74°, and three energies (200 eV, 500 eV, and 1000 eV). The experimental angular distributions compare very well with the calculated distributions; the mean percentage deviation between them was about 10% at 200 eV, and decreased to about 5% at 1000 eV. Agreement between theory and experiment was not improved when DCSs determined from muffin-tin potentials were used in the calculations. This result justifies the use of DCSs for isolated atoms in theoretical description of elastic-electron backscattering from surfaces.
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Keywords: Computer simulations; Electron–solid interactions; Electron–solid scattering and transmission-elastic; Monte Carlo simulations; Electron spectroscopy; Amorphous surfaces

1. Introduction

Analytical techniques founded on measurements of the elastic-electron backscattering intensity are known by the acronym EPES (elastic-peak electron spectroscopy) [1–3]. A frequent application of such technique is the determination of the electron inelastic mean free path in the surface region of solids [1]. This method is recognized as the only experimental source providing IMFPs which agree with the ASTM definition [4] of this parameter. The relevant experiment consists in measurements of the elastic-peak intensity in a particular experimental configuration, and the IMFP value is obtained after fitting the calculated intensity to the measured intensity. It is of crucial importance to use in calculations a reliable theoretical model that describes well the phenomenon of elastic backscattering from solids in different experimental configurations.

A useful test of validity of the theoretical model, describing the elastically backscattered intensity, is a comparison of the experimental angular distribution of elastically backscattered electrons with the calculated distribution. Such a comparison has been made already in 1970 by Schilling and Webb [5] in studies of electron elastic backscattering from liquid mercury. These authors developed a relatively simple analytical theory taking into account multiple elastic collisions in the solid. It has been shown in later works that the

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doi:10.1016/j.susc.2006.07.011

angular distribution of elastically backscattered electron is well described by Monte Carlo simulations of electron trajectories in the solid [6–8]. There are also analytical theories describing elastic-electron backscattering; however the relevant formalism becomes very complicated [8–11]. In computational practice, the Monte Carlo simulations presently seem to be the most accurate and convenient in determination of different characteristics of backscattered electrons, in particular, in calculations of the angular distribution. The drawback of this approach is the relatively large computational effort that is needed to reach a reasonable accuracy. A prospective approach is the recently proposed trajectory-reversal algorithm which exhibits relatively fast convergence [12].

Measurements of the elastic-backscattering probabilities for determination of the IMFP can be performed in different experimental configurations. As follows from a compilation of such configurations [1], the primary beam was incident along the surface normal in practically all published reports. The emission angles varied in a wide range depending on the configuration of the spectrometer: from 20° to 70° in the case of small acceptance angle analyzers, or between 5° and 55° in the case of integrated signal by the retarding field analyzers. If a theoretical model is reliable, the resulting IMFP should not depend on the experimental geometry. This issue has been approached by Jablonski and Jiricek [13] who determined the IMFPs for Si, Cu, Ag and Au from elastic-backscattering probabilities measured for emission angles ranging form 5° to 45°. Noticeable variation of the IMFPs were observed for emission angles smaller than 25°. These effects were ascribed to the deficiency of the theoretical model. In a recent work [14], two Monte Carlo strategies were compared: conventional simulation and the trajectory-reversal simulation. It was found that these algorithms lead to insignificant differences. It is also well known that the differential elastic-scattering cross sections (DCS) originating from different sources may considerably affect the resulting IMFPs [3]. This issue is also approached in detail in the present work.

In all theoretical models describing the effect of elastic backscattering, the DCSs used in calculations were calculated for isolated neutral atoms. Obviously, the potential describing the interaction between an electron and an isolated atom and the potential between an electron and atom inside a solid must be different. Preliminary calculations of the DCSs for the muffin-tin potential, simulating a solid, indicate that they are different from the DCSs calculated for neutral atoms [15,16]. Furthermore, the use of the DCSs from the muffin-tin potential and DCSs from the potential for the isolated atoms leads to differences in the resulting attenuation length values [17], although this difference is not very pronounced. An obvious question arises if the theoretical models for elastic-electron backscattering from solids based on the DCSs calculated for the muffin-tin potentials are more accurate than the models using the DCSs calculated for neutral atoms. To answer this question, we compare here the elastic-backscattering probabilities calculated using different DCSs with the elastically backscattered intensities measured in different experimental geometries.

2. Experimental

2.1. Spectrometer

The elastic-peak spectra were recorded with an angle-resolved photoelectron spectrometer ADES 400 (VG Scientific, UK) equipped with an electron gun (Varian, model 981-2455), Mg Kα (1253.6 eV) and Al Kα (1486.6 eV) X-ray sources, and a rotatable hemispherical electron energy analyzer. In the reported measurements, the analyzer was operated in the FAT mode at a pass energy 100 eV for XPS or 20 eV for EPES. The electron-beam current was 0.1–1.0 μA, and the electron-beam diameter at the sample surface was ~3 mm. The electron elastic-backscattering intensities were recorded at primary-electron kinetic energies of 200 eV, 500 eV, and 1000 eV. During measurements, the electron-beam incidence angle was normal to the sample surface, while the emission angles were varied by rotation of the analyzer between an emission angle of 35° with respect to the surface normal and an emission angle of 74°. Elastically backscattered electrons were collected by the analyzer within a small conical acceptance angle. The half-cone angle of the analyzer was 4.1°. The experimental geometry was carefully checked by a laser beam technique.

2.2. Samples

Elastic-backscattering intensities from Si, Fe, Co, Ni, Cu, Pd, Ag, Sm, Ir, and Au samples were measured in all experimental geometries considered. Before the EPES measurements, all sample surfaces were sputter-cleaned until no traces of contamination were seen in the XPS spectra. The typical width at half maximum of the elastic peak in the applied energy range was $\leqslant$0.5 eV. The inelastic-electron background was subtracted using Shirley's procedure. The silicon sample was a Si(1 1 1) wafer cut from a Si single crystal and polished. The surface roughness was evaluated to be below 1 nm. The samples of Fe, Co, Ni, Cu, Ag, Ir and Au were metal overlayers deposited on the Si(1 1 1) substrate. This procedure ensured high smoothness of the sample. The thickness of the deposited layer was in the vicinity of 400 nm, and was controlled during deposition by a crystal quartz monitor. This thickness made possible further sample processing, i.e. amorphisation by sputtering prior to EPES measurements.

The polycrystalline palladium and samarium samples were polished metal foils: palladium (99.9%, Goodfellow, UK) with a thickness of 0.5 mm, and samarium (99.9%, Safina, Czech Republic). There were some experimental problems with removing oxygen from the samarium sample. After prolonged sputtering, the oxygen signal became very small, although still visible. We estimate the final oxygen concentration as several atomic percent.

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