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Photoinduced $KL_{23}L_{23}$ Auger transitions in Ge thin films

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Abstract

Ge $KL_{23}L_{23}$ Auger spectra photoexcited (using bremsstrahlung radiation) from thin Ge films were measured with high energy resolution. The measured spectra were corrected for effects of inelastic electron scattering within the films, using two different models for estimating inelastic backgrounds. From the corrected Auger spectra the relative transition energies, the relative intensities and the energy widths of the $KL_{23}L_{23}$ Auger lines were evaluated and compared to earlier results obtained from X-ray induced Auger spectra, from Auger spectra emitted from radioactive isotopes and from Auger spectra induced by high energy electrons transmitted through ultrathin Ge layers.

Keywords: Auger spectra; Ge KLL; Transition energy; Relative intensity; Photoexcitation; Thin film; Electron scattering

1. Introduction

High energy resolution Auger spectroscopy of deep core transitions in atoms of materials of great practical importance provides unique possibilities for analyzing the depth and chemical state resolved composition of the constituents non-destructively at buried interfaces as well as for revealing the electronic structure local to the initial state core hole. In the case of semiconductors used as particle or photon detectors, the precise knowledge of the core Auger spectra is important for the better understanding of the response of these detectors to X-rays.

Earlier works, including the KLL Auger transitions in a Ge film using Mo Kα radiation for excitation [1], the Ge KLL spectra emitted from ^{73}Ge radioactive isotope atoms following the nuclear decay of ^{73}As isotopes through electron capture [2] and the Ge KLL spectra induced by high energy electrons transmitted through ultrathin Ge layers [3] determined the transition energies and the relative intensities for the respective Auger lines. A strong satellite line was identified in these spectra as a consequence of inelastic electron processes in the Ge films. Our recent study [4] indicates a significant (30–40%) contribution of intrinsic plasmon excitation (due to the appearance of the core holes) to this satellite, in addition to the contribution of inelastic electron scattering (extrinsic plasmon excitation). It is important to clarify the effect of these phenomena on the quantitative evaluation of photoinduced Ge KLL Auger spectra. In addition, the comparison of the Auger spectra induced by photons from a thick Ge layer (detection of Auger electrons in backscattering geometry) to the Auger spectra induced by electrons from ultrathin layers (detection of Auger electrons in transmission geometry) can lead to interesting new information on the contribution of inelastic electron scattering to the spectra due to Auger and excitation processes in Ge. Comparing the photoinduced Ge KLL Auger spectra to the Ge KLL spectra emitted from ^{73}Ge atoms created in the decay of ^{73}As, the possible effects of the different initial states of the Auger process can be studied. In the radioactive decay of the ^{73}As isotopes, an electron is captured into the nucleus producing a vacancy in the 1s shell and as a consequence, the nuclear charge is decreased. At the same time an outer shell electron finds itself excited to an unoccupied electronic state. Because both the atomic number (nuclear charge) and the number of electrons in the atom have decreased by the same quantity, during the nuclear decay process the atom remains neutral. The electron capture process is then followed by various relaxation processes in the excited neutral atom including rearrangements of atomic electrons, shake up/off or other phenomena taking place within the atomic shells. On the other hand, in the case of core photoionization, due to the photoexcitation a photoelectron is produced leaving the atom with a core hole as a positive ion. Photoionization is accompanied by simi-

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lar electronic rearrangements as in the case of electron capture. Concerning Auger transitions in Ge atoms following electron capture in ^{73}As or photoionization of Ge therefore the electron configurations in the respective initial states are different. In the ^{73}Ge excited atom there is a vacancy in the 1*s* shell and there are three electrons in the 4p shell while in the photoionized Ge atom there is a vacancy in the 1s shell and two electrons in the 4p shell.

2. Experimental

Polycrystalline Ge layers of ca. 100 nm thickness were vacuum deposited onto Si wafers using a d.c. magnetron and a quartz crystal microbalance for monitoring the thickness of the deposited layer. Prior to electron spectroscopic studies, the surfaces of the samples were cleaned in situ using Ar ion sputtering, removing the surface contamination layer of less, than 1 nm thickness. Ge $KL_{23}L_{23}$ Auger spectra were excited from the Ge layers by Cu X-rays (bremsstrahlung) and were measured using our high energy ESA-31 electron spectrometer [5] based on a 180° hemispherical deflector energy analyzer, applying an energy resolution of 2.6 eV at 8500 eV electron energy. For energy calibration of the spectrometer in the high energy range Cu 2p and Cu 3s lines excited by Cu Kα radiation from pure Cu metal samples, were used [6]. Reflection electron energy loss (REELS) spectra obtained from the Ge surfaces were measured using 8000 eV primary electron energy and the same energy resolution, an angle of incidence of 50° for the exciting electron beam and an angle of emission of 0° for the detected electrons [4].

3. Evaluation of the measured Ge KLL auger spectra

Evaluating the measured spectra first the contribution, attributable to electrons scattered inelastically in the sample (the inelastic background), was removed. For this purpose, two different methods were used.

3.1. Method A

After correcting for a constant background component, the contributions from extrinsic electron energy losses were removed using the method based on the analysis of the inelastic tail of the Auger lines [7] and the corresponding QUASES-Tougaard software [8] developed by Tougaard, applying the cross-section for inelastic scattering of electrons within the solid as derived from the measured REELS spectra [9]. The QUASES-Tougaard method (and algorithm) is based on the following equation describing the primary (excitation or source function) spectrum $F(E)$ emitted from the atoms embedded in a homogeneous solid:

$$F(E) = J(E) - \lambda_i \int_E^{\infty} K(E' - E) J(E')\,\mathrm{d}E'$$

where $J(E)$ is the measured spectrum, $K(E' - E)$ the cross-section for inelastic scattering, derived from the measured REELS spectra and λ_i is the mean free path for inelastically scattered electrons. The spectra left following inelastic background correction were fitted by Auger peaks having asymmetric Lorentzian shape and by a tail describing the contribution of electrons suffered energy losses in intrinsic type processes. The Lorentzian shape energy distribution was asumed for the electron energy loss function concerning intrinsic type losses and a Poissonian distribution was assumed for multiple intrinsic losses according to the model of Hüfner [10].

3.2. Method B

Using this method, the contributions due to electrons suffering bulk and surface type energy losses were removed from the spectrum step by step with an iterative procedure, applying the Partial Intensity Analysis (PIA) method developed by Werner [11]. The PIA model describes the emitted spectrum $Y(E)$ as [11]:

$$Y(E) = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \sum_{n_3=0}^{\infty} C_{n_1 n_2 n_3 \ldots} F_{n_1 n_2 n_3 \ldots}(E)$$

where the C_{n_i} partial intensities—i.e. the number of the particles participating n times in the *i* type of loss process, are derived by Monte Carlo simulation [14] of the elastic and inelastic scattering, while the corresponding partial energy loss distributions $F_{n_1, n_{2\ldots}}(E)$ are obtained convolving the primary peak by energy loss functions of the individual processes [11]. For bulk and surface losses, the respective electron energy loss functions were derived from experimental optical data [12], in the case of bulk losses the effects of momentum transfer were taken into account according to Penn [13]. Calculating the partial intensities and the Surface Excitation Parameter for surface losses the respective material parameter was taken from Ref. [15]. The spectra left following these corrections were fitted by a model spectrum generated according to the formula above. For energy distribution of the elastic (primary) peak a Doniach-Sunjic type function was used. The partial energy loss distribution for a single intrinsic loss process was approximated with an asymmetric Lorentzian function. For intrinsic partial intensities, a Poissonian distribution was used. This procedure is different from that used in Ref. [16] for describing intrinsic losses assuming an energy loss function with the same shape as for bulk losses, as well as determining the contribution from electrons suffered intrinsic type energy losses by an adaptive fitting [16].

4. Results and discussion

The measured photoexcited Ge KLL spectra and the results of evaluation of the measured spectra using different models for inelastic background correction are shown in Figs. 1–4 and the KLL transition energies, relative Auger peak intensities and the energy widths (Full Width at Half Maximum, FWHM) of the Auger peaks derived from these evaluations are presented in Tables 1–3.

The measured Ge $KL_{23}L_{23}$ spectrum, excited from a polycrystalline Ge layer of 100 nm thickness, using Cu bremsstrahlung, can be seen in Fig. 1. As a consequence of the