Corrected electron inelastic mean free paths (IMFPs) for selected wide band semiconductors

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Abstract. Elastic peak electron spectroscopy (EPES) has been widely used to determine the electron inelastic mean free paths (IMFPs) in solids. In this work, we investigated quantitatively the influence of surface excitations on electron IMFPs determined by EPES. We used IMFPs obtained from the early EPES measurements of the electron elastic backscattering probability from GaN and Cd_{0.88}Mn_{0.12}Te wideband-gap semiconductors, and the Ni standard in the energy range 200–2000 eV. The total surface-excitation parameter (SEP) was evaluated using Chen and Werner approaches, and was applied for correcting the EPES IMFPs. These corrected values were then compared with those predicted by the TPP-2M formula. We found that implementation of the surface-excitation correction improved agreement between the resulting IMFPs for selected wide band semiconductors and the TPP-2M values at low-energy (E < 500 eV) electrons. The extent to which the IMFPs measured by EPES differ from the corresponding bulk values (on account of surface excitations) was found to depend on the semiconductor material with finite surface. Our results also clearly demonstrated the importance of accounting for surface excitations for accuracy of the IMFPs measured for GaN.

1. Introduction
The problem of surface excitations in different applications of surface analysis by electron spectroscopies has been extensively studied [1-3]. In addition, improvement in quantitative surface analysis was found to be significant when surface excitations were considered. Such excitations are usually characterized by the so-called surface-excitation parameter (SEP), which describes the total probability of surface excitations for both incident and escaping electrons from the solid [4].

A widely used experimental method to determine the electron inelastic mean free path (IMFP) in solids is the application of elastic-peak electron spectroscopy [1,5]. Principles of relative EPES measurement procedures have been already described in details elsewhere [1,5]. However, this method requires correction for the surface-excitation effect in order to determine absolute values of IMFPs or when the measurement were made without standard. To obtain reliable quantitative information from EPES spectra, the measured intensities and/or peak areas should be corrected for these effects.

In the present work, measured EPES IMFPs in the wideband semiconductors GaN [6] and Cd_{0.88}Mn_{0.12}Te [7] are corrected for surface excitations using Chen [4] and Werner et al. [8] corrections, and compared to Tanuma et al. [9] predictive IMFPs.
2. Surface-excitation corrections

Details of relative EPES measurements used here in calculations of SEPs have been recently published by Krawczyk et al. [6,7]. Briefly, the experimental configurations used for determining the EPES IMFPs have been the following: incidence angle $\alpha_{\text{in}} = 0^\circ$, emission angle $\alpha_{\text{out}} = 42.3^\circ$, electron energy range $E = 200-2000$ eV for GaN with respect to Ni standard [6]; incidence angle $\alpha_{\text{in}} = 0^\circ$, emission angle $\alpha_{\text{out}} = 60^\circ$, electron energy range $E = 500-2000$ eV for Cd$_{0.88}$Mn$_{0.12}$Te with respect to Ni standard [7]. In the case of gallium nitride, experimental IMFPs refered to the Ga$_{60}$N$_{50}$ sample with a thin surface layer enriched in Ga (~70 at.%) [6].

Different methods were proposed to account for surface excitations in electron spectroscopies [1,4,8,10-12]. Since in EPES analysis the electron crosses the surface twice, the total surface-excitation parameter, $P_s(E, \alpha)$, (SEP) for incoming, $P_s(E, \alpha_{\text{in}})$, and outcoming, $P_s(E, \alpha_{\text{out}})$, electrons of energy $E$, and both incident angle $\alpha_{\text{in}}$ and escaping angle $\alpha_{\text{out}}$ with respect to the surface normal can be expressed as [13]

$$ P_s(E, \alpha) = P_s(E, \alpha_{\text{in}}) + P_s(E, \alpha_{\text{out}}) $$

(1)

In this work, the SEP, which describes the influence of surface excitations by electrons for the vacuum side in electron spectroscopies, were calculated for electrons of 200-2000 eV energies crossing surfaces of GaN, Cd$_{0.88}$Mn$_{0.12}$Te and Ni. These calculations were performed for both incident and escaping electrons by the use of two approaches of Chen [4] and Werner et al [8].

Chen [4] determined a general formula for $P_s(E, \alpha)$ using a free-electron-gas model together with the surface energy-loss function. The SEP for metals and semiconductors can be conveniently fitted as [4]:

$$ P_s(E, \alpha) = a_{\text{Ch}} E^{-1/2} \cos^{-1} \alpha, $$

(2)

where the electron energy $E$ is in eV, $a_{\text{Ch}}$ is a material-dependent fitting parameter. The parameter $a_{\text{Ch}}$ is found to be 4.55, 2.98 and 2.84 for GaN, Cd$_{0.88}$Mn$_{0.12}$Te and Ni, respectively.

Werner and coworkers [8] proposed a simple analytical expression for describing the SEP in different materials:

$$ P_s(E, \alpha) = 1/(0.173a_{\text{H}} E^{1/2} \cos \alpha + 1), $$

(3)

where $a_{\text{H}}$ is a material-dependent parameter. From the present calculations, $a_{\text{H}}$ is found to be 0.17, 0.27 and 0.31 for GaN, Cd$_{0.88}$Mn$_{0.12}$Te and Ni, respectively.

The total surface-excitation factor $f_s$ can be described as [14]:

$$ f_s = \exp[-P_s(E, \alpha_{\text{in}})] \exp[-P_s(E, \alpha_{\text{out}})]. $$

(4)

To introduce the surface energy losses into the theory of elastic backscattering, we need to multiply the EPES-measured ratio of elastic-backscattering probabilities by the surface electronic excitation (SEE) correction $K = f_s^{\text{sample}}/f_s^{\text{standard}}$.

3. Results and discussion

Since in relative EPES measurements for GaN [6] and Cd$_{0.88}$Mn$_{0.12}$Te [7] semiconductors no surface effects were considered, we corrected EPES-measured elastic-peak ratios for surface-excitation processes.

In Figures 1 and 2, the SEP dependencies on energy are displayed for GaN and Ni, and also for Cd$_{0.88}$Mn$_{0.12}$Te and Ni, respectively, using Chen [4] and Werner et al. [8] approaches. Although the shapes of energy dependencies are similar, pronounced differences are mainly found for GaN and Ni (Figure 1).
In case of both considered semiconductors, the Werner SEP [8] values are higher in the energy range 500-2000 eV. For nickel, we observe that the resulting SEPs are very similar. The present results show that small differences exist in the SEPs for Cd$_{0.88}$Mn$_{0.12}$Te semiconductor and Ni (similar inelastic-scattering properties) but large differences occur between GaN semiconductor and Ni. These results clearly indicate that the SEP corrections for GaN cannot be neglected, especially at low electron energy (E < 500 eV), and should be appropriately corrected.

Figure 1. Energy dependence of the total SEP calculated for GaN and Ni using Chen and Werner SEPs. $\alpha_{in} = 0^\circ$, $\alpha_{out} = 42.3^\circ$.

Figure 2. Energy dependence of the total SEP calculated for Cd$_{0.88}$Mn$_{0.12}$Te and Ni using Chen and Werner SEPs. $\alpha_{in} = 0^\circ$, $\alpha_{out} = 60^\circ$.

Figure 3. Comparison of IMFPs for GaN measured by EPES using Ni standard. Solid line: IMFPs from the TPP-2M formula [9].

Figure 4. Comparison of IMFPs for Cd$_{0.88}$Mn$_{0.12}$Te measured by EPES using Ni standard. Solid line: IMFPs from the TPP-2M formula [9].
Figures 3 and 4 compare the corrected EPES IMFPs with EPES IMFPs without correction for the surface energy losses in both the studied semiconductors. These values are also compared with values predicted by the TPP-2M formula [9]. We notice that the corrected IMFPs are still close to the Tanuma et al. data. For GaN, differences between the corrected and as-measured data are pronounced for all energies studied (Figure 3). The corrected data are systematically above the Tanuma et al. values. Except for energies of 200 and 1500 eV, the corrections applied here lead to rather worse results with respect to the bulk-like data. For Cd$_{0.88}$Mn$_{0.12}$Te (Figure 4), however, results of the EPES IMFP values uncorrected as well as corrected are in close vicinity.

4. Conclusions
Two approaches to the surface-excitation parameter (Chen, and Werner et al.) were applied for wideband GaN and Cd$_{0.88}$Mn$_{0.12}$Te semiconductors. The SEPs calculated here were then used for correction of the electron elastic backscattering probability, and finally to obtain the EPES IMFPs. The results show that small differences exist in SEPs among Cd$_{0.88}$Mn$_{0.12}$Te and Ni but large differences occur between the values for GaN and those for Ni. We conclude that SEP corrections for GaN cannot be neglected, especially at low electron energy (E < 500 eV), and should be appropriately corrected.

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