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Monte Carlo simulations of electron transport in solids: applications to electron backscattering from surfaces

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Abstract

We report results of Monte Carlo simulations to investigate the effects of backscattered electrons in scanning Auger microscopy (SAM) on the radial distributions of emitted Auger electrons. We considered the emission of copper M_3VV and L_3VV Auger electrons from a thin Cu overlayer on a substrate of silicon or gold for primary electrons with energies of 5 and 10 keV that were normally incident on the sample. The Cu layer was assumed to be sufficiently thin that there were no changes in the angular and energy distributions of primary and backscattered electrons passing through the overlayer. We report values of the information radius, r_a^P, from which a selected percentage P of the emitted Auger electron intensity originates. Values of r_a^P found here range from 119 Å (Cu $L_3M_{45}M_{45}$ Auger transition, $E_0 = 5$ keV, Au substrate, $P = 80$) to 6757 Å (Cu M_3VV Auger transition, $E_0 = 10$ keV, Si substrate, $P = 95$). For the same substrate, primary energy, and chosen value of P, values of r_a^P are larger for Auger electrons from the Cu M_3VV Auger transition than for the Cu $L_3M_{45}M_{45}$ Auger transition. In addition, values of r_a^P increase with primary energy and are larger for the Si substrate than the Au substrate. The values of r_a^P are generally much larger than the radius of the primary beam (assumed to be 50 Å here) on account of inner-shell ionizations by backscattered electrons. We also report values of the mean escape radius, $\langle r \rangle$, that range from 82.5 Å (Cu $L_3M_{45}M_{45}$ Auger transition, $E_0 =$ 5 keV, Au substrate) to 1169 Å (Cu M_3VV Auger transition, $E_0 = 10$ keV, Si substrate). Knowledge of r_a^P and $\langle r \rangle$ is important in the analysis of fine features in SAM because appreciable Auger signal can be collected from the nearby region as well as from the feature of interest. Finally, we report Monte Carlo simulations of Auger line scans across the edge of a thin Cu overlayer on a Si or Au substrate. The shapes of the line scans depended only weakly on the Cu Auger transition, although the differences were more pronounced for the Si than the Au substrate. On account of backscattered electrons, the lateral distance corresponding to

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signal variations of 25% and 75% of the maximum intensity in a line scan varied from 53.6 Å (Cu $L_3M_{45}M_{45}$ transition, E_0 = 5 keV, Si substrate) to 75.1 Å (Cu M_3VV transition, E_0 = 10 keV, Au substrate).

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1. Introduction

The lateral resolution in scanning Auger electron microscopy (SAM) is mainly determined by the diameter of the electron beam incident on a specimen surface. In commercially available modern spectrometers, this diameter may be smaller than 10 nm. However, it is known that, due to the transport of incident electrons in the specimen, the area from which detected Auger electrons are emitted may considerably exceed the beam diameter. In recent work, Powell [1] studied the SAM analysis area using a simple analytical model to describe the lateral distribution of Auger electron emission for normally incident primary electrons. This model, introduced originally by Cazaux [2,3], is based on the assumption that the radial distribution of Auger electrons emitted in a given direction is the sum of two Gaussian functions: one describing emission of Auger electrons arising from inner-shell ionizations by the primary incident on the surface, and the other describing Auger electron emission arising from similar ionizations by backscattered electrons.

A more accurate description of the lateral distribution of Auger electron emission requires Monte Carlo simulations of electron trajectories in the surface region. Such calculations have been published by several groups [4–6]. The objective of the present work is to report results of similar calculations based on the development of a reliable Monte Carlo algorithm for calculations of the radial distribution of Auger electron emission. In our physical model, the latest developments in electron transport theory are introduced.

We present simple analytical expressions in Section 2 for possible radial distributions of the primary beam and for the radial distribution of emitted Auger electrons. The Monte Carlo simulation algorithm is described in Section 3, and we present and discuss our results in Section 4. We first show radii of the analysis areas for Cu M_3VV and L_3VV Auger electrons from thin films of copper on silicon and gold substrates with excitation by 5 and 10 keV primary electrons. We then show simulated line scans for Cu M_3VV and L_3VV Auger electrons as the primary beam was scanned across the edge of a thin Cu film on silicon and gold substrates, again with excitation by 5 and 10 keV primary electrons. For both applications, we show how backscattered electrons can affect the analysis area and the line scans. We conclude with a summary in Section 5.

2. Radial distribution of the Auger electron signal intensity

Let us consider a substrate covered by a very thin overlayer film. We will calculate the Auger electron signal from a selected film material (here Cu) on substrates of Si and Au. The overlayer material is assumed to be sufficiently thin so that the energy and angular distributions of backscattered electrons calculated for the substrate material are not modified significantly by the presence of the film; that is, the distributions for the substrate will apply to the film. We also assume, for simplicity, that the surface is bombarded by a focused electron beam (the primary beam) along the surface normal.

It is convenient to describe the radial distribution of Auger electron emission by a function providing the Auger electron current per unit area as a function of the radial distance, r, from the beam axis. This function, denoted by $J_A(r)$, is normalized so that

$$I_{max} = \int_0^\infty 2\pi r J_A(r)\,dr \tag{1}$$