PHOTOELECTRON EFFECTS ON THE DOSE DEPOSITED IN MOS
DEVICES BY LOW ENERGY X-RAY SOURCESD.B. Brown
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A method for calculating electron transport in layered materials is described. It is applied to a problem of radiation damage in MOS capacitors irradiated with a Cu x-ray tube operated at 45 kV. The effects of photoelectron transport are found to be significant. A problem of energy deposition in x-ray lithography is also discussed. The dose in the SiO₂ gate is found to be about equal to that in the x-ray photoresist. Electron transport effects are found to be small in this lithography problem.

INTRODUCTION

There are a number of problems where it is necessary to know in detail the depth distribution of energy deposited by relatively low energy photon sources. For example, Dozier et al. have suggested that the investigation of radiation effects in MOS devices can usefully be performed using such a source, in particular a Cu target x-ray tube operated at 45 kV (1,2). In order to properly interpret the data obtained using such a source it is essential to treat the effect of photoelectron transport on the depth profile of energy deposition in the test device. In this paper we shall present such a treatment, based on a numerical solution of the Boltzmann equation. The methods to be described will be based on the previous work of Brown and co-workers (3,4,5,6,7) where they have been extensively applied to problems of x-ray production and x-ray analysis in the 1-10 keV regime.

In addition, it has been suggested that fine-line lithography might be obtainable using x-ray sources of somewhat lower energy, for example, a rotating Al anode tube operated at 10 kV (8,9). We shall apply our techniques to the calculation of the dose-depth profile in a model x-ray lithography problem.

The methods to be described are less expensive than Monte Carlo treatments of energy deposition in layered media. In addition they are less approximate than the diffusion treatment of Garth (10).

In the remainder of this paper we shall (a) discuss a simplified approach to the Cu tube deposition problem, (b) discuss a more refined treatment of the same problem and (c) discuss the Al tube (lithography) problem.

TREATMENT OF MONOENERGETIC PHOTOELECTRONS

The problem at hand can be treated usefully in a somewhat simplified form. We begin by establishing the rationale for this simplified model. Figure 1 shows (in dashed lines) a calculated dose profile for a MOS capacitor. This dose profile was obtained by taking into account photoelectric absorption of the incident photons while ignoring electron transport effects. It is useful to think of it as the energy deposition which exists after photon absorption has taken place, but before any electron transport has taken place. The correction of this curve for electron effects is, then, the principal subject of this paper. In Fig. 1 the dose in each layer has been normalized to that in SiO₂, for simplicity. The indicated deposition was caused by a commercial Cu target x-ray tube operated at 45 keV with a .025 gm/cm² thick Ni filter used to eliminate

eliminate most of the Cu K β line. The spectral output of the tube was obtained using a program developed by J.W. Criss (11). The output of this program has been shown to be in agreement with experimental data and with the prediction of more elaborate programs (6,7). We must now consider what spectrum of electrons will be generated by the deposited energy shown in Fig. 1.

The energy deposition of Fig. 1 may be broken up into contributions from the various energies in the incident filtered Cu x-ray tube spectrum. The contribution from the Cu K α line, at about 8 keV, constitutes 78% of the deposited energy. Of this energy deposited by Cu K α photons, the majority must end up as photoelectrons of energy (8-E_K) keV, where E_K is the K shell ionization energy for the element being ionized. The highest K shell ionization energies to be considered are those for Al and Si which are about 1.7 keV. If we allow for the fraction of energy which is absorbed by L and higher shell ionization and for the energy carried away by Auger electrons, it follows that greater than 64% of the deposited energy is transferred to photoelectrons of >6.3 and <8 keV. There will be some electrons of lower energy (mainly Auger electrons) and some of higher energy (mainly photoelectrons resulting from the high energy bremsstrahlung component of the x-ray tube). In summary, it will be a first approximation to assume that all of the deposited energy is transferred to electrons with a kinetic energy of 7 keV.

ELECTRON TRANSPORT THEORY

We will now consider how the transport of these 7 keV electrons within a layered medium may best be handled. We shall describe an approach which, to our knowledge, has not previously been applied to "interface effects," though it is a close relative of the work of Garth (10). That is, Garth's diffusion approximation is a limiting case of the more general approach we will describe.

Brown et al. (3,4) have treated related problems with the numerical solution of the equation

$$(\partial/\partial s) \sin\theta f(x, \theta, s) = -\cos\theta (\partial/\partial x) \sin\theta f(x, \theta, s) + \{1/\lambda(s)\} (\partial/\partial \theta) \{\sin\theta (\partial/\partial \theta) f(x, \theta, s)\} \quad (1)$$

In Eqn. 1 the distribution function, $f(x, \theta, s)$, is the probability that an electron which has traveled a distance s will have a position between x and $x+dx$ (measured from the surface) while its direction of travel has an angle between θ and $\theta+d\theta$ (measured from the internal surface normal). If both sides of Eqn. 1 are divided by the stopping power dV/ds , we may produce a second equation which is now in terms of a differential in energy rather than a differential in path length,

$$(\partial/\partial V) \{\sin\theta f(x, \theta, V)\} = - (ds/dV) \cos\theta (\partial/\partial x) \{\sin\theta f(x, \theta, V)\} + (ds/dV) \{1/\lambda(V)\} (\partial/\partial \theta) \{\sin\theta (\partial/\partial \theta) f(x, \theta, V)\}. \quad (2)$$

It can be shown (4) that when the electrons become sufficiently isotropic, then Eqn. 2 may be approximated by

$$(\partial/\partial V) D(x, V) = (ds/dV) \{\lambda(V)/6\} (\partial^2/\partial x^2) D(x, V) \quad (3a)$$

where

$$D(x,V) = 2\pi \int f(x,\theta,V) \sin\theta d\theta \quad (3b)$$

Eqn. 3a, which has the form of a diffusion equation, has been applied by Garth (10) to the problem of interface effects (it is his Eqn. 12). In Eqns. 1-3 the parameter λ is the transport, or momentum transfer, mean free path. In comparing the utility of the three equations given above we may summarize:

1. Eqn. 1 is not simply applicable to layered media. This is because the electrons in the various layers do not have a single energy for a given value of s , leading to difficult numerical problems.

2. Eqn. 3 has the advantage of simplicity and of simple analytical solutions under some conditions, as discussed by Garth (10).

3. Eqn. 2 is, in general, more accurate than Eqn. 3. In addition, for the problem here considered, it is found to be more than an order of magnitude cheaper to obtain a numerical solution of Eqn. 2 than to obtain one of Eqn. 3. A brief explanation of this fact is as follows. The large gradients in electron density found near interfaces in MOS devices tends to cause instability in the numerical solution. The second derivative with respect to depth of Eqn. 3a is more sensitive to this problem than is the first derivative with respect to depth of Eqn. 2. Such instabilities are eliminated by shifting to a finer subdivision of the energy (smaller ΔV) with an attendant increase in computation effort. It should be emphasized that there are problems for which the diffusion equation is cheaper. One such case has been described in Ref. 4.

4. Because of its superior accuracy, and because it is a straightforward matter to apply a numerical solution method to layered media, we have chosen to use Eqn. 2.

Equation 2 has been solved by transforming it into difference equations which yield a value of $f(x,\theta,V)$ at $V-\frac{1}{2}\Delta V$ from four values of $f(x,\theta,V)$ at V , and then calculate a value of $f(x,\theta,V)$ at $V-\Delta V$ using four of the values of $f(x,\theta,s)$ just calculated for $V-\frac{1}{2}\Delta V$. This scheme is iterated, beginning with the initial value of V and continuing to a lower cutoff energy. The low energy cutoff is chosen to be as high as possible (to minimize computation cost) but sufficiently low that a little shift in the electron density profile occurs below this energy. The size of the voltage interval is chosen to be as large as possible (to minimize computation cost) but sufficiently small that the numerical solution does not become unstable. At the initial energy a two dimensional array representing $f(x,\theta,V)$ is given a set of values representing the initial electron distribution. The angular range is divided into 11 intervals ($\Delta\theta = \pi/10$), while the depth is divided into 42 intervals. An elementary discussion of the numerical methods used can be found in, for example, Ref. 12. The solution algorithm is embodied as a computer program currently running on a DEC PDP-10. Additional discussion of the application of this program can be found in Refs. 3-6.

MONOENERGETIC SPECTRUM - RESULTS

We shall now consider the application of the transport calculation just described to our problem of 7 keV electrons deposited in an MOS structure. The energy deposition process shown first in Fig. 1 by the dashed lines is shown again in Fig. 1 by the solid lines, this time after the electron transport has been completed. Similar calculations have been performed for four additional SiO₂ thicknesses (250, 750, 3000 and 20000 Å). Figure 2 shows as solid lines the energy deposition in the oxide as a function of position

within the oxide for each of the five oxide thicknesses treated. Note that the 7500Å curve represents the same data previously shown in Fig. 1. In addition, similar calculations have been performed for the same five oxide thicknesses using a gate of Si rather than one of Al. Figure 2 also shows the energy deposition in the oxide for these Si gate capacitors (dashed lines).

Note that the degree of dose enhancement in the oxide is strongly dependent on oxide thickness. It is also dependent on the gate material, reaching a maximum of about a factor of 1.65 for the Al gate and a factor of 1.8 for the Si gate. These results are not greatly affected by electron loss at the gate-vacuum interface, at least for the gate thicknesses used here.

USE OF A POLYCHROMATIC ELECTRON SPECTRUM

The calculations described in the previous section were much simplified by the assumption of a monoenergetic electron spectrum. We shall now outline a more rigorous approach. A realistic polychromatic spectrum was obtained in the following manner. The x-ray tube spectrum is obtained using the Criss program, as described above. This spectrum is input into a photon transport code which does five things. First, the spectrum (including both lines and bremsstrahlung) is broken into a histogram. Second, this histogram spectrum is deposited into a layered specimen, using standard x-ray absorption coefficients (13). Third, the absorbed energy is partitioned among the elements and the several ionizations (K,L,LI, etc.) using standard absorption coefficients and absorption edge jump ratios (13). Fourth, the energy associated with a given ionization is partitioned among photoelectrons, Auger electrons, and photons. We have used the fluorescence yield factors of Bambynek et al. (14). Fifth, an electron spectrum data file is produced for later use by electron transport programs.

The result of the above series of calculations as applied to the filtered 45 keV Cu tube spectrum in SiO₂ is shown in Fig. 3. For the cases treated in this paper a negligible fraction of the absorbed energy is transferred to characteristic line photons, i.e., the majority of the energy is transferred to photoelectrons and Auger electrons.

An electron spectrum such as that of Fig. 3 can be introduced into a solution of Eqn. 2 in a straightforward manner. As the solution steps down through the range of electron energies, additional electrons are introduced as appropriate. The Auger electrons were given an isotropic angular distribution. The photoelectrons were given a $\sin^2\theta$ distribution (15). It was determined that the results were insensitive to the angular distribution assumed for the photoelectrons. Figure 4 shows how the results of Fig. 1 are modified by the introduction of this more realistic spectrum. It can be observed that the differences between using 7 keV electrons and using a more realistic electron spectrum are in this case noticeable, but small.

ENERGY DEPOSITION IN X-RAY LITHOGRAPHY

In this section we shall treat a second example where energy deposition in layered materials is of current interest. In the attempt to develop a workable x-ray lithography technique, two important considerations are the energy deposition in the photoresist and in the SiO₂ layers (8,9,16). We have applied the methods described above to a representative x-ray lithography problem. As a typical x-ray source we have assumed a rotating Al anode x-ray tube at 10 kV. As a typical specimen, we have taken a structure consisting of 5000 Å of PBS (photoresist), 1000 Å of SiO₂, 5000 Å of polysilicon and 1000 Å of SiO₂ (gate), on a Si substrate.

The results of our dose calculations are given in Fig. 5. The dashed line represents the deposition which would be calculated from photon absorption alone. The solid line gives the results of the full calculation including the effects of photon absorption (for x-ray line and bremsstrahlung) and electron transport (photoelectrons and Auger electrons). Two conclusions can be drawn from Fig. 5. First, the dose in the SiO₂ gate is about the same as the dose in the PBS photoresist. This implies a considerable radiation damage problem, as has been previously observed (16). Second, the deposition profile is dominated by the photon absorption effects. The effects of electron transport are (in this case) second order effects, except perhaps within the infinitesimal regions adjacent to the interfaces. (A complementary discussion of this point has been given in Ref. 8.)

CONCLUSION

This paper has demonstrated a calculation of energy deposition profiles in realistic device structures at kilovolt energies. The degree to which electron transport effects modify the energy deposition in MOS structures is quite dependent on the problem under consideration. We have shown that for deposition due to a 45 kV Cu x-ray tube the dose enhancement can approach a factor of two. On the other hand, the effects found using a 10 kV Al x-ray tube are small except within a few tens of Angstroms of the interfaces.

The series of computer programs containing the algorithms demonstrated above provide a useful tool for the evaluation of dose effects in layered materials in the 0.5 to 50 keV region. They are relatively simple and inexpensive to use. They have been tested by comparison with experimental data (3-7). They could be extended to treat high energies by adding Compton electron effects. To accomplish this the program which calculates the photoelectron and Auger electron distributions would be replaced by a more elaborate photon transport program.

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Fig. 1. Dose distribution in an MOS capacitor irradiated by Cu x-ray tube operated at 45 kV.

Fig. 2. Dose in oxide vs. oxide thickness for Al gate (—) and Si gate (----) MOS capacitors.

Fig. 3. Histogram electron spectrum calculated for SiO_2 irradiated by a Cu x-ray tube operated at 45 kV.

Fig. 4. Effect of a more realistic electron spectrum.

Fig. 5. Energy deposition in a model x-ray lithography structure caused by an Al target x-ray tube operated at 10 kV.