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TRIM SIMULATIONS AND POSSIBLE STUDIES FOR EDGE-ON ION IRRADIATION OF ELECTRON MICROSCOPE SPECIMENS*

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ABSTRACT

A TRIM code [1] has been modified to simulate a special technique, first described at the Spring 92 MRS Meeting [2], for in situ transmission electron microscope (TEM) experiments involving simultaneous ion irradiation, in which the resultant phenomena are observed as in a cross-section TEM specimen without further specimen preparation. Instead of ion-irradiating the film or foil specimen normal to the major surfaces and observing in plan view (i.e., in essentially the same direction), the specimen is irradiated edge-on (i.e., parallel to the major surfaces) and is observed normal to the depth direction of the irradiation. The results of calculations utilizing the modified TRIM code are presented for cases of 200 and 500 keV Co impinging onto the *edge* of Si films 200 and 600 nm thick. The limitations of the technique are discussed and the feasibility of experiments involving implantation of Co into Si and the formation of $CoSi_2$, which employ this technique, are briefly discussed.

INTRODUCTION

Common practice when in situ ion irradiation experiments in a TEM are performed is to observe the specimen and hence the resulting phenomena in plan view, the irradiation and viewing directions being more or less normal to the surface of the specimen. Furthermore because of the requirement that TEM specimens must be relatively thin (several tenths of µm and substantially less for heavy metals), deep implantation-type experiments, for example, have not been possible in situ. Rather, following irradiation and usually subsequent heat treatment, a cross-section TEM (XTEM) specimen is prepared in order to analyze the material microstructure. Although quite laborious, this is a very useful and powerful technique for obtaining a lot of information from a single specimen, information which may be directly correlated to other techniques such as Rutherford Backscattering Spectroscopy (RBS). XTEM techniques have largely replaced the much more laborious and oftentimes uncertain "sectioning" techniques involving carefully controlled thinning of bulk irradiated material from the irradiated side to a desired depth, followed by backthinning to produce the electron transparent region corresponding to that depth. Such sectioning techniques required multiple specimens with identical irradiation and thermal histories. In principle at least, the specimen preparation problems associated with the XTEM and other sectioning techniques can be circumvented by performing an in situ TEM experiment in which the specimen is ion irradiated at 90 degrees with respect to the TEM viewing direction; i.e., the ion irradiation is incident on an edge of the specimen, parallel to, rather than normal to, the major surfaces of the specimen. The ideal disposition of the specimen with respect to the electron and ion beams for this situation is depicted in Fig. 1. This turns the specimen into a kind

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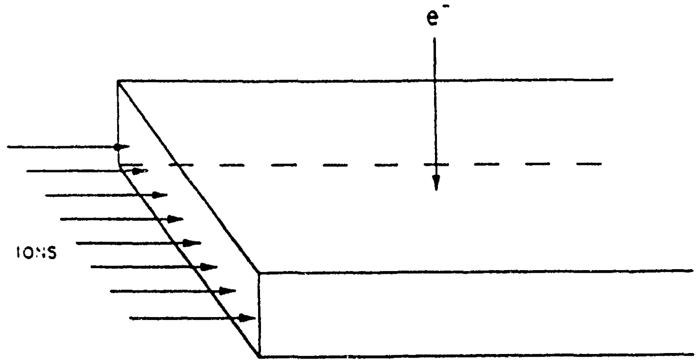

Fig. 1. Ideal configuration for in situ TEM experiment involving edge-on ion irradiation with simultaneous TEM analyses.

of dynamic cross-section specimen as far as the observer is concerned. The advantage of this is that the time evolution of resultant phenomena is available, so that a single specimen serves the purposes of a series of XTEM specimens in a particular irradiation experiment. The chief disadvantage of this edge-on geometry, of course, is that there are two free surfaces in one of the directions which is lateral with respect to the incident ion beam. In order to assess the experimental conditions under which these free surfaces do not dominate the course of resulting phenomena, a conventional TRIM (transport of recoils in metals) simulation has been modified to take account of the finite lateral dimension of the bombarded specimen. The purposes of this paper are to describe this program modification briefly and to present characteristic results of calculations for the edge-on implantation of Co ions into Si films for two ion energies and two specimen thicknesses. Finally, because the simulation assumes no migration of atoms or defects following displacement events, the additional limitations to the proposed experimental technique, arising from the finite mobilities of atoms during real experiments of the deep implantation-type, are assessed.

TRIM SIMULATION

The simulation of ion irradiation experiments for the geometrical situation depicted in Fig. 1 is based on TRIM 90, the source code for which was supplied by Ziegler [3]. The graphics were stripped from the source code and the program adapted to the Macintosh. The essential adaptation of the program to this problem is threefold. First, one of the lateral dimensions (y-direction), which in standard TRIM is infinite, is restricted to finite values corresponding to the thickness of the TEM specimen. Second, this thin specimen is imagined to be composed of a number of slices normal to the y-direction, as shown in Fig. 2; the x-direction is the inward normal of the surface onto which the ions are incident. Third, the ions impinge on the specimen edge at $x = 0$, at positions random in y. In standard TRIM the numerical output of a simulation ignores, of course, the y-distributions of defects and implanted atoms, which are essentially uniform if the material is not finite in y, and presents only information with respect to depth x from the surface of incidence. In our problem the y-distributions as well as the x-distributions are important so that the output has also been modified to yield the x-distributions *within* each of the slices. The results which are presented here are for y-slice thicknesses $\Delta y = 10$ or 30 nm and an x-direction calculation depth of 1 μm (that is, the calculation increment $\Delta x = 10$ nm). The results for implantation of Co ions of two energies, 0.2 and 0.5 MeV, incident on Si films of two thicknesses, 200 and 600 nm, are discussed. Because the number of y-slices in both cases is 20, the slice thickness $\Delta y = 10$ nm for the 200 nm thick film and 30 nm for the 600 nm film. Each simulation involves a total of 100,000 ions incident on the

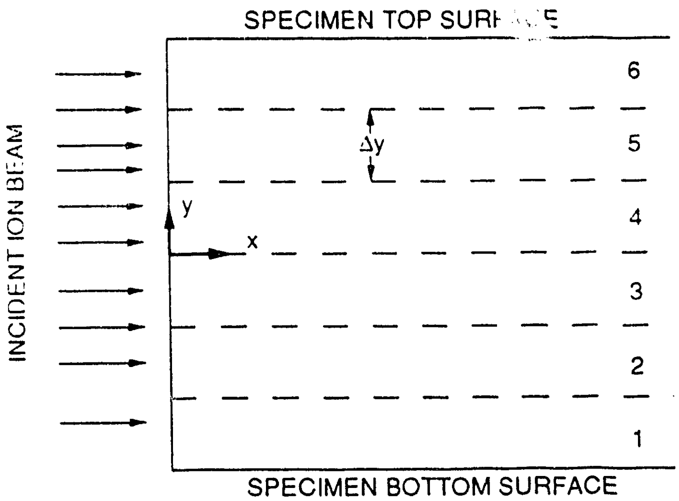

Fig. 2. Thin film with ion beam incident onto edge of film. For computational purposes, film is divided into slices, Δy thick, normal to y-direction. Ion incidence is random with respect to y.

specimen edge at $x = 0$ (random incidence with respect to y). With a Mac IIFX, the machine times for the implantation calculations range from about 11 hours for 200 keV Co ions on the edge of a 200 nm Si film to about 36 hours for 1500 keV ions on a 600 nm film. In these calculations, no account has been taken of sputtering of the front surface, which can overwhelm other effects during low temperature implantation [4].

After verifying that calculated results are the same within statistical limits for corresponding y-slices equidistant from the center of the film (for example, the pairs 1-6, 2-5 and 3-4 in Fig. 2), the output results of the distributions of implanted Co for each of these y-slice pairs are summed. The results are normalized so that the graphical output shows Co ions implanted (per 100,000 Co ions incident on the edge of the specimen) within a given y-slice pair per increment Δx as a function of x.

At the present time the y-slice thickness Δy is not an independent input parameter of the modified TRIM program, but is the specimen thickness t divided by 20; i.e., there are always 20 y-slices. The main reason for this seemingly arbitrary choice is the limited capacity of the Mac II to accommodate a significantly larger amount of output data, the amount increasing in proportion to the number of y-slices.

The implantation results from the TRIM calculations for the two incident ion energies and two film thicknesses are presented in Fig. 3. Each graph includes the implanted Co distributions for all ten of the y-slice pairs, that for the outermost pair (slices 1 and 20) being the lowest curve in each case. The quantity I is the fraction of ions implanted in the film.

<u>200 keV Co on Edge of 200 nm Si Film (Figure 3a)</u>

The y-slice thickness $\Delta y = 10$ nm. Clearly the y-slices at the surfaces (lowest curve) have retained less than half as much Co as the innermost y-slices. The behavior of the first 30 nm from each surface is noticeably different from the remaining 70 percent of the film. However, of the total number of ions incident on the film edge, 89 percent have been implanted.

<u>200 keV Co on Edge of 600 nm Si Film (Figure 3b)</u>

The y-slice thickness $\Delta y = 30$ nm. The distribution of implanted Co in the two y-slices nearest the surfaces are easily distinguished from the distributions in the other y-slices. Note that these two y-slice pairs in this case represent a total of 120 nm of the

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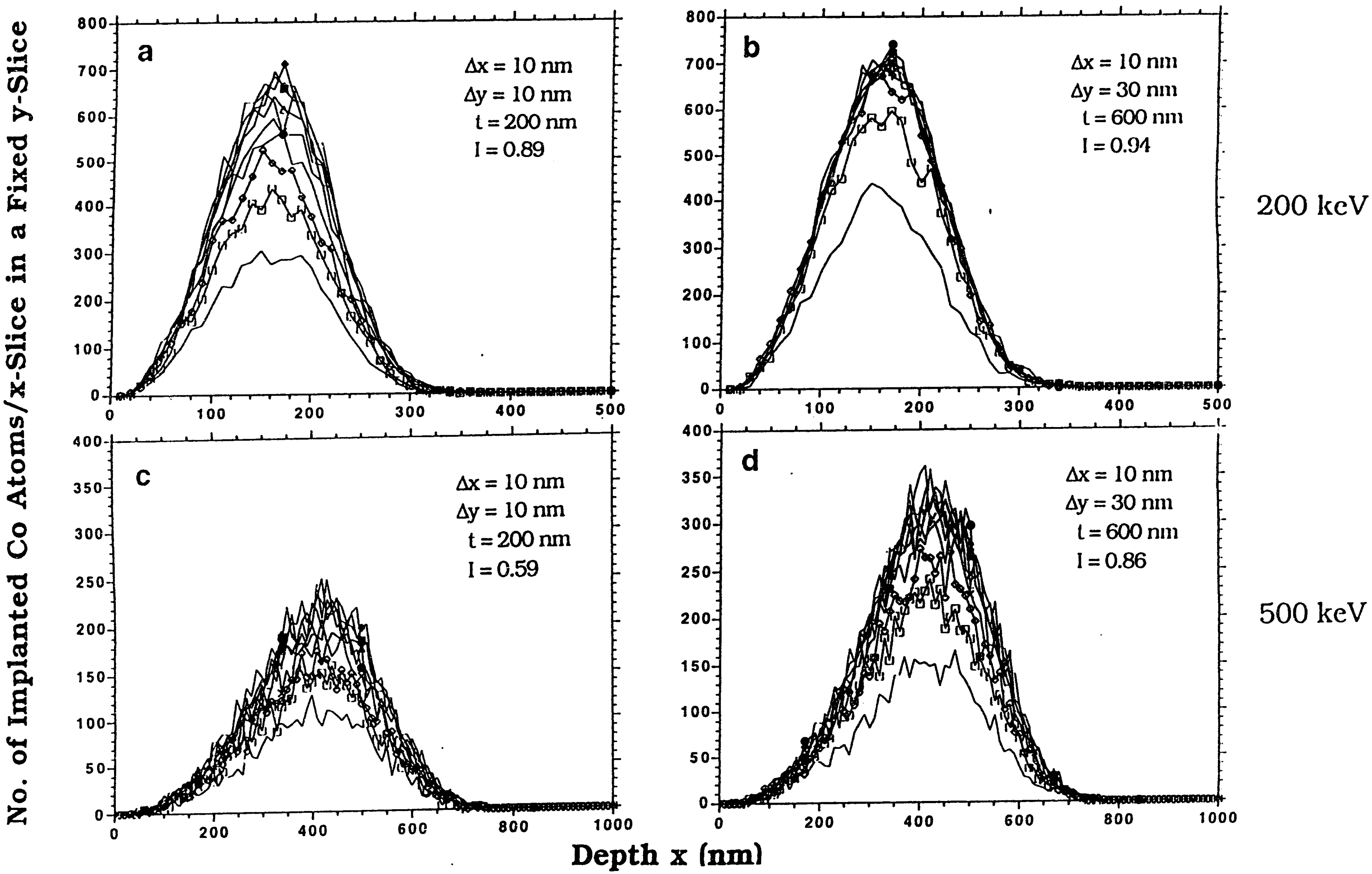

Fig. 3. Modified TRIM simulations of implantation of Co during edge-on irradiation of Si by (a)(b) 200 and (c)(d) 500 keV Co for specimen thicknesses t of (a)(c) 200 and (b)(d) 600 nm. In each graph the lowest curve is the implanted Co distribution in the y-slices nearest the bottom and top surfaces (1+20). I = fraction of Co implanted.

film so that the Co distributions in 80 percent of the film are virtually identical. In this thicker film 94 percent of the incident Co has been retained.

<u>500 keV Co on Edge of 200 nm Si Film (Figure 3c)</u>

The y-slice thickness Δy = 10 nm. Clearly the y-slices at the surfaces (lowest curve) have again retained less than half as much Co as the inner y-slices. The behavior of the first 30 nm from each surface is noticeably different from the remaining 70 percent of the film. Of the total number of ions incident on the film edge, only 59 percent have been implanted.

<u>500 keV Co on Edge of 600 nm Si Film (Figure 3d)</u>

The y-slice thickness Δy = 30 nm. The distribution of implanted Co in the three y-slices nearest the surfaces are easily distinguished from the distributions in the other y-slices. Note that these three y-slice pairs in this case represent a total of 180 nm of the film, which is almost the thickness of the Si film described in Figure 3a, consistent with the magnitudes of the numbers of Co atoms implanted. In this thicker film, however, 86 percent of the incident Co has been retained.

There is very little, if any, difference between the implanted Co distributions within the inner y-slices corresponding to Figs. 3(a), (b) and (d) and those from standard TRIM calculations. There is a significant difference for 500 keV Co on a 200 nm film of Si, however, as is clear from a comparison of Figs. 3(c) and (d).

FEASIBILITY OF SUCCESS OF EDGE-ON IMPLANTATION EXPERIMENTS

The implantation of Co into bulk Si has been widely studied by both RBS and XTEM [4–8]. There still remain questions, nevertheless, regarding the specific sequence of events during the formation, ripening and ultimate coalescence of $CoSi_2$ precipitate crystals. Such implantations must be performed at an elevated temperature such as 620 K or higher in order to prevent amorphization of the Si. Furthermore the development of the silicide is usually accomplished by subsequent annealing at still higher temperatures rather than implanting at such temperatures (850–1400 K, for example). Co is a fast diffuser in Si [9]. Ref. 9 does not present data for Co, but on the assumption that the diffusivity is similar to that for Cu and Ni, one would conclude that at 700 K, for instance, the diffusivity is 10^{-10} to 10^{-11} m^2 s^{-1}. For implantations requiring one hour, one would estimate that Co implanted early in the process at 700 K could migrate roughly 1 mm in one hour if in solid solution. In fact, of course, $CoSi_2$ layers form at reasonable implant depths, suggesting that nucleation of the silicide readily occurs as a consequence of the very low equilibrium solubility of Co in Si, thus immobilizing the Co. An alternative explanation comes from Hashimoto et al. [10], whose diffusivity data for Co in Si indicate that Co is a fast diffuser only at sufficiently high temperatures, such as 1200 K and above, but the activation enthalpy is much greater than those of regular fast diffusers such as Cu, Ni, Li and Fe [9] and D_0 is anomalously large. Consequently the diffusivity of Co, obtained by a long extrapolation of the high temperature data to 700 K, yields a diffusivity of the order 10^{-20} m^2 s^{-1}. This would reduce the diffusion distances, as estimated above, by 5 orders of magnitude or more and clearly changes the complexion of the problem. The edge-on implantation of Co into a Si film seems worth the effort, therefore, especially for a relatively thick film (e.g., 600 nm) and incident ion energy of 500 keV or less. Such an in situ experiment can be readily performed in the HVEM at Argonne's HVEM-Tandem Facility, with which the microstructural evolution can be followed by intermittent observation, employing 1 MeV electrons in conjunction with the relatively thick Si film (intermittent in order to avoid any substantial electron damage). Higher energy implantation may also be suitable, but the distribution of implanted Co will be less uniform across the film thickness and the implantation efficiency (the fraction implanted I in Fig. 3) is decreased. Results of such an edge-on in situ ion irradiation experiment involving the partial amorphization of Si by 1.0–1.5 MeV Kr bombardment have been discussed previously [2].

OTHER OUTPUT OF MODIFIED TRIM SIMULATIONS

In addition to the distribution of ion ranges presented here, the modified TRIM program will compute all the usual quantities of TRIM 90, including damage distributions. The calculation of the distribution of ion ranges presented above is relatively rapid because only the ion trajectory is determined. On the other hand, the calculation of damage distribution in each slice is more time-consuming; for example, for ten thousand 1.5 MeV Co ions on a 600 nm thick Si film, which is sufficient for reasonable statistics, the computational time for a Mac IIFX is about 48 hours. In general, especially for higher energy implants, the distributions of damage are less uniform across the film thickness for a given depth than are the implanted ion distributions. It might prove interesting to utilize this difference to examine the effects of different damage rates for a given implantation rate.

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