CONF-850813--2

DE85 016931

Paper for the

11th INTERNATIONAL CONFERENCE ON ATOMIC COLLISIONS IN SOLIDS

Washington, D.C., August 4–9, 1985

(Proceedings to be published as a Special Issue of

NUCLEAR INSTRUMENTS AND METHODS IN PHYSICS RESEARCH)

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SOLID STATE DIVISION
OAK RIDGE NATIONAL LABORATORY
Operated by
MARTIN MARIETTA ENERGY SYSTEMS, INC.
Under
Contract No. DE-AC05-84OR21400
With the
U. S. DEPARTMENT OF ENERGY
OAK RIDGE, TENNESSEE

July 1985

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ABSTRACT

Damage profiles in crystalline silicon produced by light (B) and heavy (Bi) ions with energies from 10 to 100 keV were studied using the computer program MARLOWE (version 12). The program follows not only the incident ion collision by collision, but also any Si target atom that is set into motion through an energetic collision. Thus, the transport effect of the complete cascade of recoiled target atoms is included in the damage profile. The influence of channeling was studied for Si(100) using beam tilt angles from the surface normal of 0°, 3° and 7° about the [001] or [011] axes. The effects of channeling on the damage profile are twofold: first, there is a large reduction of the central damage peak; second, there is a component of the damage profile that extends considerably deeper into the target than that found in conventional studies using a random target assemblage. The influence of amorphous overlayers of SiO_2 on the damage and implantation profiles in the Si(100) substrate has also been investigated.

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*Research sponsored by the Division of Materials Sciences, U. S. Department of Energy under contract DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc.

The use of ion implantation for the controlled introduction of dopants into semiconductors has stimulated much interest in the lattice damage introduced by the implanted ions [1 and references therein]. A detailed understanding of the nature of this damage and its spatial extent is needed in order to help develop techniques to remove it efficiently [2–4]. Almost all calculations on the damage or energy loss profiles assume the slowing down of an ion in a random or amorphous medium. A major exception is the computer program MARLOWE [5,6], which treats crystalline material. In studies of ion produced damage in crystalline media, it is important to realize that ion channeling may affect the results. In channeling, the ion is constrained to move in the more open avenues of the crystal, thus greatly reducing the probability of violent collisions, which produce cascade damage. In addition, damage may be introduced at much greater depths than in an amorphous target. This can occur when long range channeled ions dechannel shortly before stopping. Effects of channeling on damage production were predicted [7] and experimentally confirmed [8] many years ago. Recently [9–11], there has been an interest in trying to characterize and quantify some of the channeling factors that affect damage production. Once these factors are quantified, it should be possible to design experiments to check the computational models and thereby gain a better understanding of the phenomena.

The present work investigated the effects of beam/crystal orientation and of oxide overlayers on the damage production in crystalline Si. The bombarding ions were B and Bi, a light and a heavy species, respectively. The calculations used the binary collision computer program MARLOWE [5,6]. The Molière [12] approximation to the Thomas-Fermi interatomic potential with a Firsov [13] screening length was used to describe the binary elastic collisions. The (nonlocal) electronic slowing down theory of Lindhard et al. [14] was used for the inelastic energy losses. In the simulation program the incident ion is followed collision-by-collision in the crystalline silicon target until it either leaves the target or slows down below 15 eV. A typical run consisted of 600–2000 incident projectiles. Thermal displacements of the target atoms were included using the Debye model. In addition to following the incident ion, any Si target atom that is set into motion when it receives an energy greater than the displacement energy E_d (15 eV) is followed until its energy drops below E_d. A lattice binding energy of 0.1 eV is assumed so that the struck atom leaves its lattice site with nearly the full transferred energy, provided it is above E_d. The spatial position of each recoil target atom together with its energy is recorded when its energy drops below E_d; from this information together with the recorded total number of interstitial-vacancy pairs produced, the number of displaced atoms as a function of depth is deduced. The interstitial-vacancy pairs included here are those whose separation distance is greater or equal to the second neighbor distance. The view is taken that the closer pairs produced will recombine. The net effect of incorporating target atom transport is to produce a damage profile at greater target depths than that deduced from the energy loss profile of the incident atom alone.

Figure 1 shows the elastically deposited energy as a function of penetration depth calculated for a 100 keV Bi ion incident at a tilt angle of 7° (about [1$\bar{1}$0] axis) from the normal of a (110) silicon surface. The dashed curve is the profile of the total elastic energy transferred by the incident Bi ion directly to the Si lattice atoms and recorded at the transfer location. The solid curve is the elastically deposited energy, taking the recoil energy transport effect of the knocked-on Si atoms into account. The figure shows that the effects of the energy transport are twofold: first there is a large reduction in the energy deposited in the surface region; second, there is an enhancement of the trailing edge of the energy deposition profile. Both of these features are due to the predominance of forward scattering experienced by the struck Si atom. Similar results have been found by Brice [15] who treated amorphous targets and included recoil energy transport in his damage calculations. Since the Si recoils also lose energy inelastically, the area under the solid curve is less than under the dashed curve. Although the tilt angle of 7° in Fig. 1 was chosen to minimize possible channeling effects (a critical axial channeling angle of 4.6° was estimated from Lindhard's channeling theory [16]), the presence of the long tail in the energy deposition indicates some channeling effects.

Figure 2 shows how the number of displaced atoms depends upon the beam direction for B incident upon a Si(100) single crystal. For each of the three cases a beam divergence of 1° was used. The tilt angle was about the [001] axis in order to minimize channeling in any of the major planes. It is seen that channeling of the incident ions greatly reduces the overall damage. In case a) where the greatest amount of channeling is expected, the overall damage is only about 40% of case c). On the other hand case b) has about 90% of the damage of case c) which indicates much less channeling than case a). This is not unexpected since the critical channeling angle [16] is estimated to be 3°. The effects of channeling on the damage profile are twofold: first, there is a large reduction of the central damage peak; second, there is a component of the damage profile that extends more deeply into the target. There are at least three reasons why damage is produced even when the beam is incident within the critical channeling angle. First, some ions never become channeled since they undergo large deflection angles in collisions with surface atoms. Second, dechanneling mechanisms, such as thermal vibrations, cause some channeled ions to dechannel before they slow down to rest. Third, it is sometimes kinematically possible for an ion to displace lattice atoms and still remain channeled. Although in the present example this is possible only while the ion is at the higher energies, it extends to lower energies when the incident ion mass is heavier than the target. The second reason and to a lesser extent the third enable the creation of damage at much greater target depths than in a random target assemblage because of the greater range of channeled ions.

Figure 3 illustrates the damage dependence of two different azimuthal angles in the beam/target orientation for 35 keV B incident upon Si(100). A beam divergence of 1° was used. Here curve a) is the same as curve c) in Fig. 2. It is seen that the peak in the damage curve b) is significantly smaller than curve a). Curve b), on the other hand shows an enhancement in the damage tail. The integrated number of displaced atoms in case b) is 78% of that of case a). The reason for the differences between the two cases in Fig. 3 is the planar channeling in case b) arising from the relatively large open (022) planes.

The effects of an amorphous oxide overlayer on the damage and projectile penetration profiles are shown in Fig. 4. An oxide layer of only 1 nm, corresponding to about four atomic layers produces a noticeable change in both profiles showing that scattering in the amorphous layer reduces the probability of ion channeling in the Si(100) substrate. When the oxide thickness is increased to 20 nm, the damage profile is qualitatively similar to an off axis tilt of 3° or 7° shown in Fig. 2. In this case it is concluded that most of the ions enter the crystalline substrate at angles that preclude channeling. It is noticed that only a small fraction of the projectiles actually stop in the oxide layer. When the oxide layer is increased from 0 to 20 nm the location of the peak in the penetration profile decreases from a depth of about 170 nm to 40 nm. This rather drastic change is due to the appreciable nuclear stopping in the latter case which is "switched" off in the former under channeling conditions. From the detailed MARLOWE output it is found that the average nuclear energy loss increases from 1/3 to 2/3 of the total energy lost as the oxide layer is increased from 0 to 20 nm. The remaining energy is lost in electronic collisions, which in the model used here, does not depend upon impact parameter.

The present study is a brief treatment of the effects of beam/target orientation and amorphous oxide overlayers on ion-produced damage in Si(100). Oxide overlayers are important, not only because of the frequency of native oxide on silicon targets, but also because similar results are expected for amorphous silicon overlayers since the masses of Si and O are similar. The latter is of interest since a proposed solution to the inadvertant ion-channeling problem in device doping is to implant first with silicon to destroy the surface crystallinity [17].

Although experimental studies on the effects of channeling on damage production have been few, there have been many studies on channeling per se. Recently, Ziegler and Lever [1] reported on an experimental mapping of the ion beam channels near the Si(100). They, as well as Michel et al. [18], find that the commonly used 7° tilt angle to insure randomness in device preparation is invalid. Their conclusions are borne out by our studies of the damage profile as shown in Fig. 3.

In conclusion, it may be mentioned that there are other factors governing channeling that will affect the damage profile. One is the divergence of the incident ion beam. It may be possible through the use of multiple scattering techniques [19] to correlate the effects of oxide overlayers to beam divergences as to their influence on the damage created in the crystal substrate.

It is a pleasure to acknowledge several fruitful discussions with John Barrett and Mark Robinson.

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FIGURE CAPTIONS

Fig. 1. The elastically deposited energy as a function of penetration depth for a 100 keV Bi ion into Si(110). The lattice constant for Si is 5.43 Å.

Fig. 2. The number of displaced atoms vs depth for 35 keV B ions into Si(100). The tilt angle gives the orientation between the beam and crystal surface.

Fig. 3. The number of displaced atoms vs depth for 35 keV B ions into Si(100) for two different tilt angles. Curve a here is the same as curve c in Fig. 2.

Fig. 4. The projectile penetration profile (left) and the damage profile (right) for 10 keV B into Si(100) with amorphous SiO_2 overlayers of various thicknesses. R_N is the fraction of B reflected from the target.

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ELASTICALLY DEPOSITED ENERGY VS PENETRATION DEPTH IN Si(110) PRODUCED BY A 100 keV Bi ION (TILT ANGLE IS 7°)

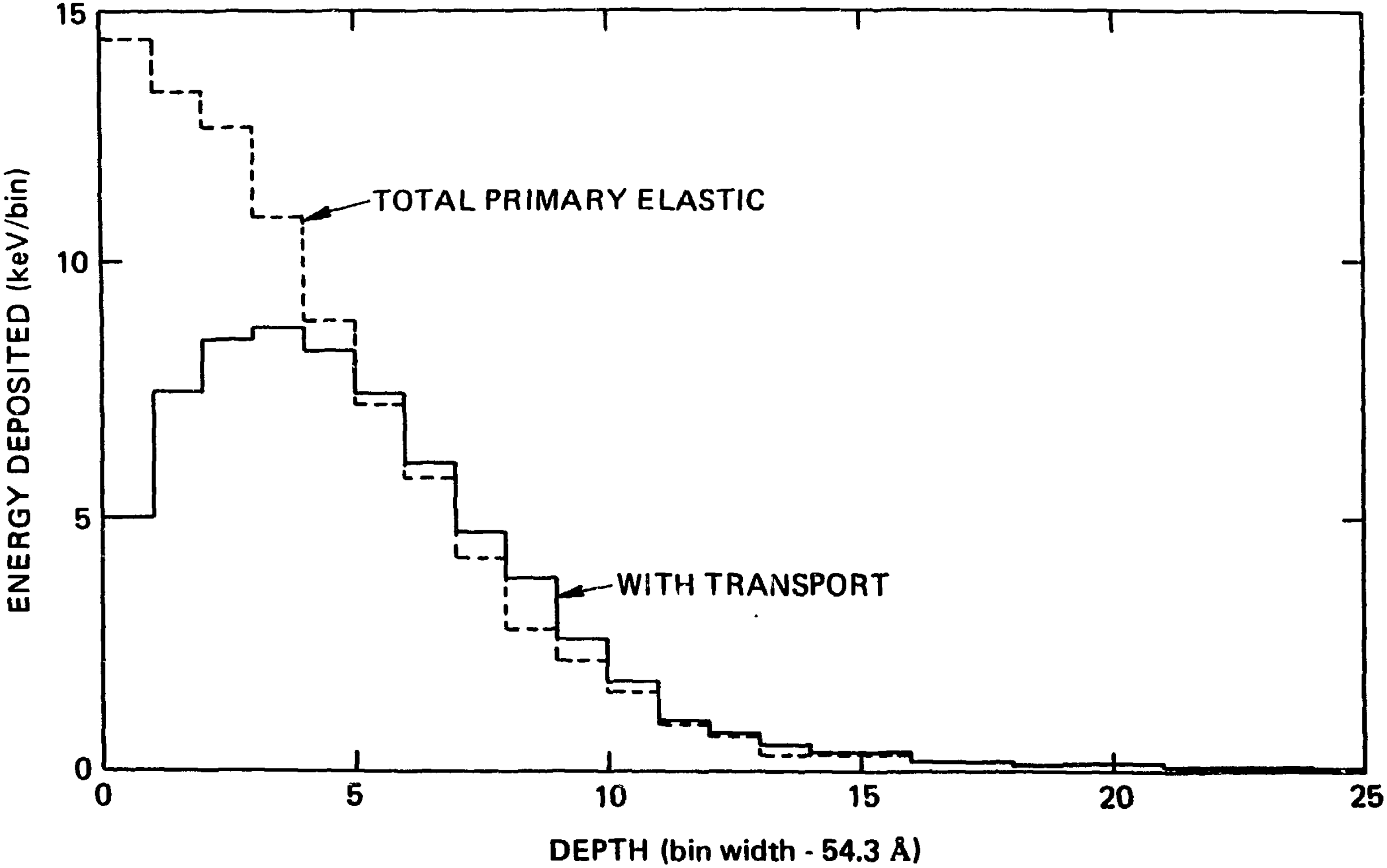

Fig. 1

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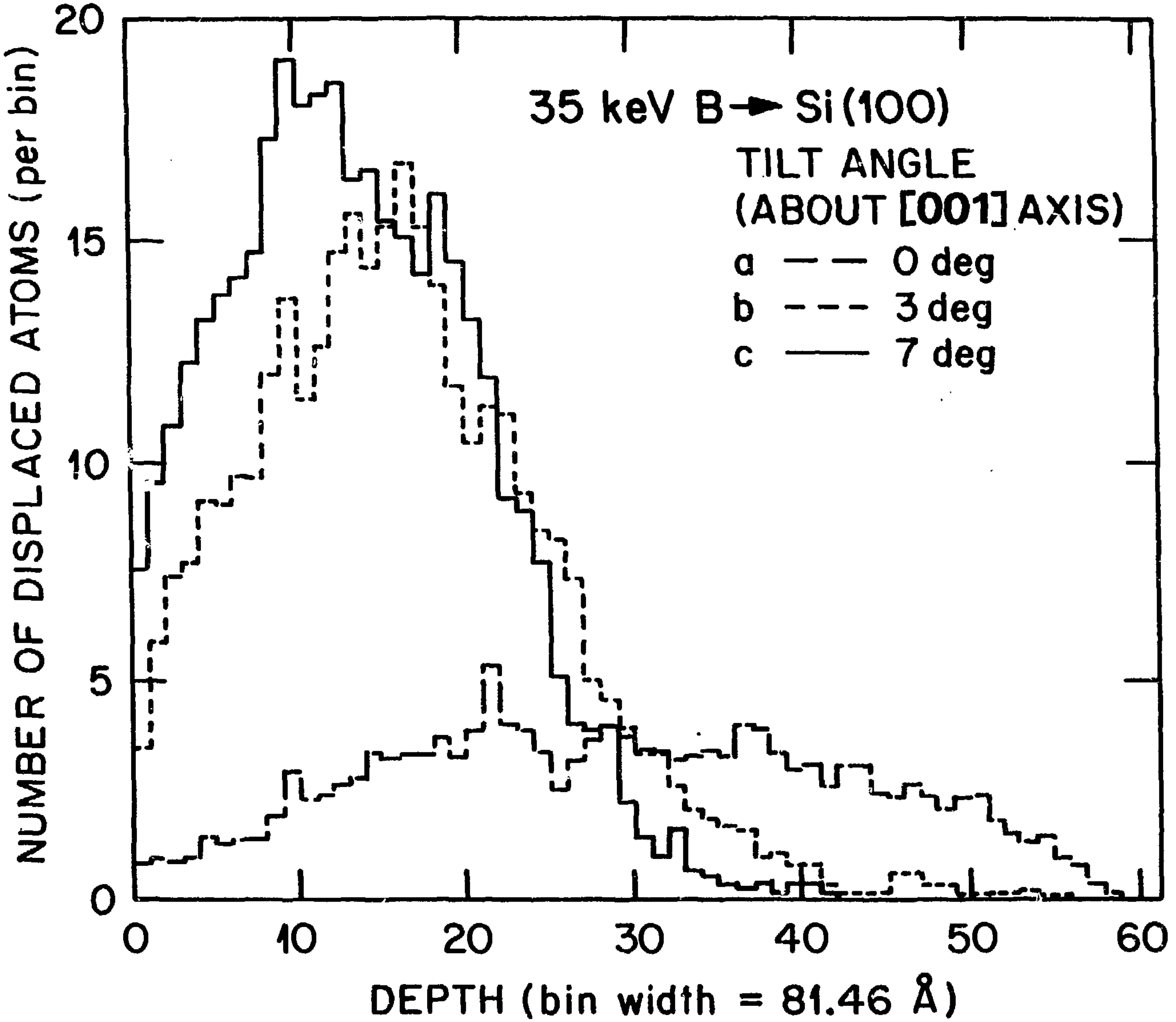


Fig. 2

ORNL-DWG 84-15170R

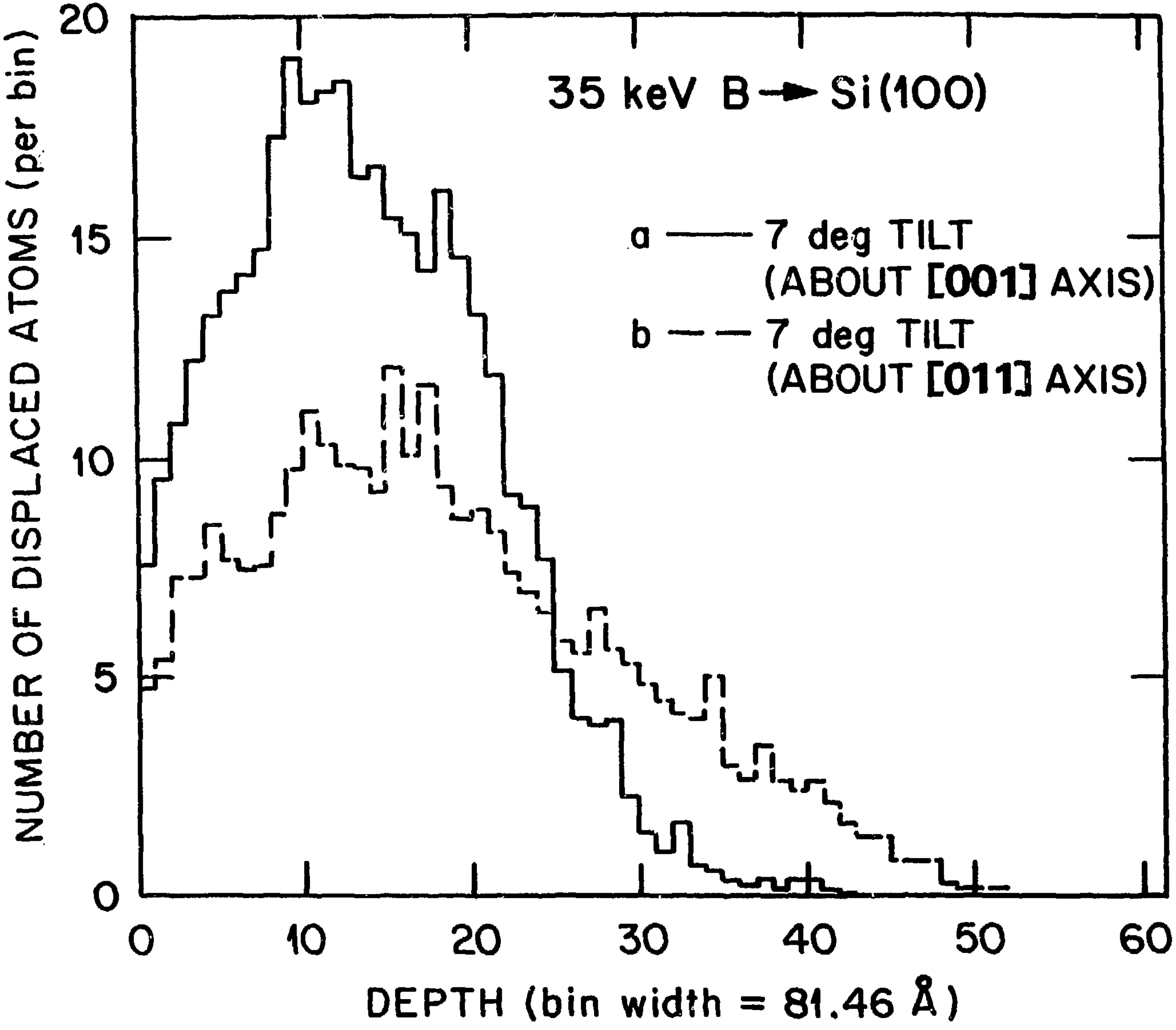
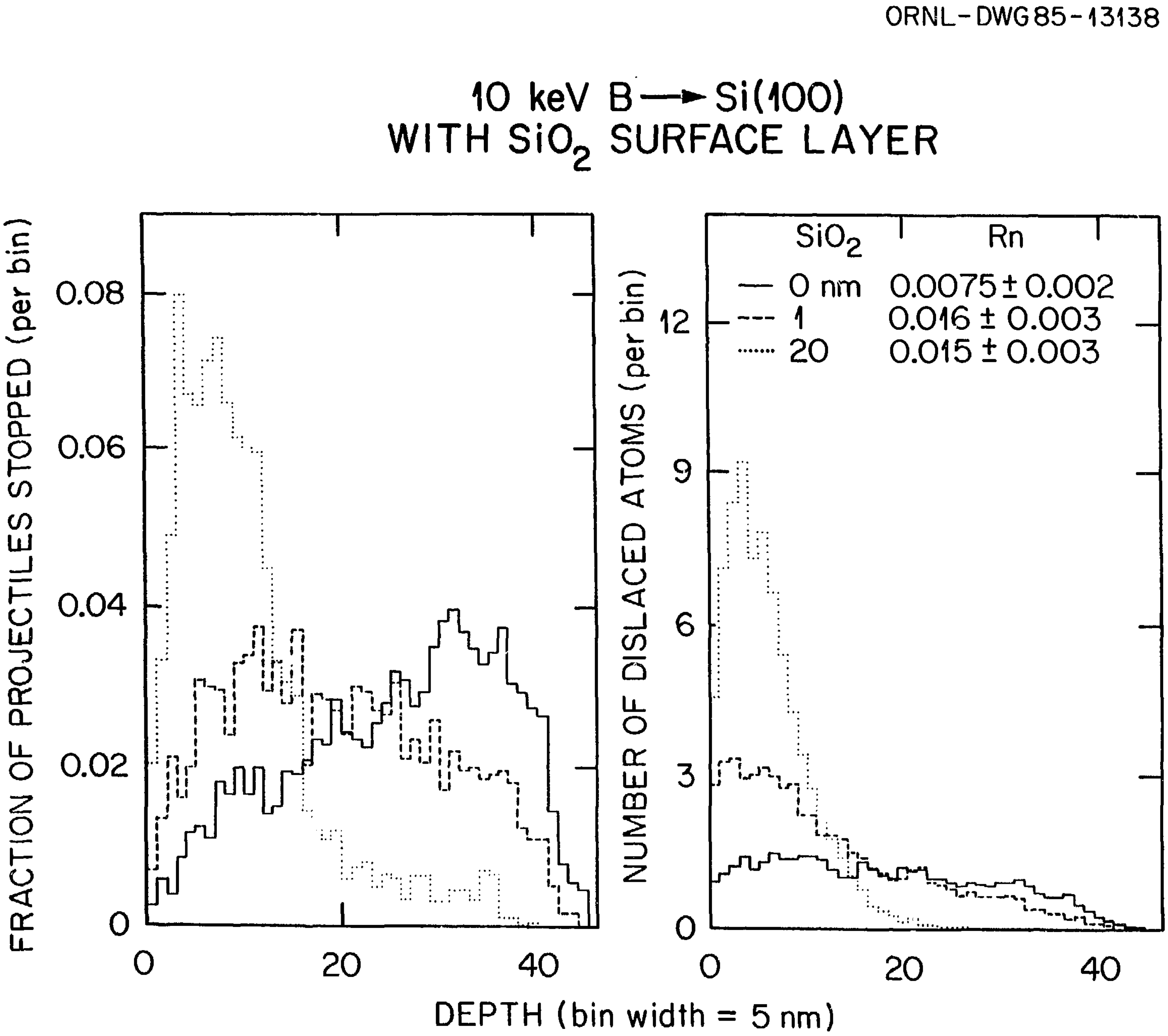


Fig. 3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10 keV B → Si(100)
WITH SiO_2 SURFACE LAYER
FRACTION OF PROJECTILES STOPPED (per bin)
0.08
0.06
0.04
0.02
0
0
20
40
NUMBER OF DISLACED ATOMS (per bin)
SiO_2
Rn
0 nm 0.0075 ± 0.002
1 0.016 ± 0.003
20 0.015 ± 0.003
12
9
6
3
0
0
20
40
DEPTH (bin width = 5 nm)

Fig. 4