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TRANSCRIPT OF THE PROCEEDINGS OF THE
FIRST ALBUQUERQUE INFORMAL RANGE/ENERGY WORKSHOP

D. F. Brice

Prepared by Sandia Laboratories, Albuquerque, New Mexico 87185
and Livermore, California 94550 for the United States Department of
Energy under Contract DE-AC04-76DP00789.

April 1981

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TRANSCRIPT OF THE PROCEEDINGS OF THE FIRST ALBUQUERQUE INFORMAL
 RANGE/ENERGY WORKSHOP

INTRODUCTION

On February 19, 1979 an informal workshop was held at Sandia Laboratories, Albuquerque, New Mexico to discuss certain aspects of the calculation of range and energy deposition distributions which are of interest in ion implantation experiments. The workshop was organized by R. M. More of Lawrence Livermore Laboratory and W. J. Choyke of the Westinghouse Research and Development Center. D. K. Brice of Sandia Laboratories was host for the meeting and is editor of the transcript.

The meeting was organized with the stated purpose "to discuss calculations of ion range, straggles, and energy deposition, with emphasis on the sizeable disagreements between results in the recent literature." It was hoped that a consensus might be reached on such questions as:

Are the disagreements real?

Which calculational approach(es) is (are) most reliable?

How reliable are they?

What further theory should/could be done to reduce the uncertainty?

What could be contributed by experiments in the near term?

This report of the workshop contains a transcript which has been edited in two stages. The editor compiled an original, edited draft of the meeting from the taped record. This rough draft of the proceedings was then circulated to each of the participants who

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had the opportunity to revise his own contribution. As can be seen from the transcript no definite consensus was reached on the last two questions in the list above, although substantive discussion on these matters did take place.

CITATIONS

This transcript is made available in order to preserve a record of the discussions at the workshop. It should not be considered as a part of the archival scientific literature, and it is therefore inappropriate to cite this report in scientific publications. Persons wishing to quote any of the information appearing here should obtain permission from the originator of the material and the citation should appear as a private communication. In this respect neither the editor, the organizers, the participants, nor the attendees at the conference makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights.

LIST OF PARTICIPANTS

H. Attaya	University of Wisconsin
R. Benedek	Argonne National Laboratory
D. K. Brice	Sandia Laboratories
W. J. Choyke	Westinghouse R & D Center
J. Ellison	University of New Mexico
L. G. Haggmark	Sandia Laboratories
R. M. More	Lawrence Livermore Laboratory
G. Mueller	Naval Research Laboratory
T. S. Noggle	Oak Ridge National Laboratory
D. Parkin	Los Alamos Scientific Laboratory
M. T. Robinson	Oak Ridge National Laboratory
J. A. Spitznagel	Westinghouse R & D Center
W. R. Wampler	Sandia Laboratories

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PROBLEMS ENCOUNTERED IN USING PUBLISHED RANGE AND ENERGY
DEPOSITION TABULATIONS

R. M. More

My remarks will be brief and to the point, and hopefully will state what the point of the workshop is. I will first remind anyone who may have forgotten what the range and range straggle are. Figure I-1 shows schematically what is meant by these two quantities. I think that in some respects the range straggle is the more important of these two quantities for people involved in ion implantation and radiation damage studies because it controls the density of the ions implanted in the target as indicated in Eq. (1).

$$N_i \sim N_{\text{Total}} / (A \cdot \Delta R_p) \quad . \quad (I-1)$$

In (1) N_i is the ion density, N_{Total} is the total number of ions implanted, and A is the surface area over which the implant takes place. So, if one wishes to relate some physical transformation in the material to the ion dose then it is important to know, or control, the range straggle. Otherwise you must change the experimental procedure so that the straggle plays a less important role, such as, for example sweeping the incident beam energy.

Jim Choyke put together some further examples of the effects of uncertainty in the straggle, and of the importance of accurately knowing the straggle in applications of the theory. Figures I-2 a-c show the calculated helium ion concentration in depth in stainless steel targets. The helium has been considered to have been implanted

at several different energies and doses in an attempt to produce a smooth distribution by overlapping the individual distributions for each separate implant energy. This was an attempt to see if one could eliminate the sensitivity of the resultant profile to the uncertainty in the straggle by sweeping the implant energy. As one can see, by comparing Figures I-2a and I-2c one can succeed or fail in this attempt if the relative straggle is altered by a factor of 2. This is almost exactly the range of uncertainties in straggle which are noted in the published values as will be seen.

Calculating the straggle involves a number of ingredients, and I have listed the most obvious of these in Table I-I. It involves information about fundamental physical processes, and there is uncertainty in these pieces of the calculation. It involves a selection of and implementation of a transport method for the calculation, and there are broadly speaking three methods of processing the atomic data, with varying degrees of accuracy. It also involves some consideration of the diffusion after stopping, and this category certainly is a contribution whose importance must be assessed in experimental measurements.

At Pittsburgh we have gathered together (See Table I-II) a set of values for the projected range and range straggle calculated by several different methods. All the data in Table I-II are for 1 MeV helium incident on solid germanium. One sees from the table that there are a number of slightly different values for the range, and several quite different values for the range straggle. The straggle values shown span a range of values of a factor of almost

two. The uncertainty of the published straggle values is thus much greater than the uncertainties in the range, and as I have indicated the straggle is possibly the more important of the two, in a practical sense. Furthermore, these numbers underestimate the true uncertainty in the straggle. In order to justify that statement it is necessary to look at what causes the straggle.

There are essentially four obvious things which cause straggle. There are 1) the random flight distance between collisions, 2) a variable angle of deflection in individual collisions (geometric effect), 3) a variable energy loss in individual collisions, and 4) an amplification of the straggle in subsequent collisions. This last is tied to the effect of the energy dependence of the stopping power on the distribution in energy of the ions. That is, for a stopping power which is a decreasing function of ion energy those ions which have less than the average energy experience a higher than average stopping power while those with more energy than average have a lower than average stopping power thus amplifying the straggle as the particles penetrate further into the material.

It is clear that the electronic energy loss contributes only negligibly to these processes, with the possible exception of (4). That is, electronic stopping only gives small angular deflections, and thus the contribution to straggle from electronic processes is primarily due to (3), i.e., a variable energy loss in individual collisions, and to (4), which are of comparable magnitude. The electronic contribution to the relative straggle from (3) is easily shown to be quite small. The precise equations governing the

the range and range straggle are

$$R(E) = \int_0^E \frac{dE'}{N_a S(E')} \quad (I-2a)$$

$$S(E) = \int T d\sigma \quad (I-2b)$$

$$\Delta R^2(E) = \int_0^E \frac{\Omega^2(E') dE'}{N_a^2 S^3(E')} \quad (I-2c)$$

$$\Omega^2(E) = \int T^2 d\sigma \quad (I-2d)$$

In Eqns. (2 and 3) R and ΔR are range and range straggle, respectively. S is the stopping cross section, N_a is the target atomic density and $d\sigma(E, T)$ is the differential cross section for energy transfer T to an electron by an incident projectile of energy E . If σ is the total cross section, $\langle T \rangle$ is the average value of T in a collision, and $\langle T^2 \rangle$ is the average value of T^2 in a collision then these equations can be approximated by

$$S = \langle T \rangle \sigma \quad (I-3a)$$

$$\Omega^2 = \langle T^2 \rangle \sigma \sim \langle T \rangle^2 \sigma \quad (I-3b)$$

$$R = \frac{E}{N_a \sigma \langle T \rangle} \quad (I-3c)$$

and

$$\Delta R^2 = \frac{\langle T^2 \rangle E}{N_a^2 (\langle T \rangle \sigma)^3} \quad (I-3d)$$

Thus,

$$\frac{\Delta R}{R} = \frac{\langle T^2 \rangle}{E \langle T \rangle}^{1/2} \sim \frac{\langle T \rangle^{1/2}}{E} = \left(\frac{1}{N_{\text{coll}}} \right)^{1/2} \quad (\text{I-4})$$

where N_{coll} is the average number of electronic collisions suffered by the projectile as it comes to rest. Since $\langle T \rangle$ is small, N_{coll} is large and thus the bottom line is that $\Delta R/R$ will be relatively small for low energy projectiles as compared, for example with the straggle due to atomic collisions. Further, the amplification effect indicated in (4) will be negative at low projectile energies, thereby reducing the electronic contribution to straggle still further.

Referring back to Table I-II all the calculations represented there assumed the same nuclear interaction, i.e., the Thomas-Fermi scattering cross section as discussed by Lindhard, Scharff, and Schiott was used in all these calculations except maybe those by Ziegler. It is a bit confusing from the data he has published just where his straggling values come from. The differences in the various calculations are only in the use of different computer codes and in the use of different forms for the electronic stopping. Four of the calculations were done with the same code, the EDEP code, however with the electronic stopping being the sole variable. One can see that in those cases the change in the electronic stopping has minor effects on the calculated range, but drastic effects on the straggle. The point of this discussion is then that the dominant contribution to the straggle comes from the nuclear interactions,

and that has not been altered in the various calculations represented in the table.

Wilson, Haggmark, and Biersack have developed a better version of the nuclear-nuclear scattering potential than the standard Lindhard Thomas-Fermi potential. It gives less small angle scattering because the potential is more strongly screened at large inter-nuclear distances, and since it gives less small angle scattering the nuclear energy loss is primarily through the large angle events. Then, that raises the straggle. The numbers they have published are 25-30% above the results using the Thomas-Fermi potential. In other words, the better the transport calculations the larger the straggle, and the better the treatment of the elastic scattering the larger the straggle is. Thus the true value of the straggle may be even higher than any listed there in the table.

So, that is the problem. The question I would like to see answered in the discussion here is, "How much of this disagreement is real?" The straggle values from some of the calculations can't be defended because there is some criticism of the methods employed there. Thus, this is not a real uncertainty. But, apart from this, how much of the disagreement in the calculations represents real uncertainty in the range straggle, and if none of it is real then what is the true uncertainty in the range straggle? What dominates that uncertainty and what is going to be done about it? Hopefully, there might be some decisive experiment, or series of experiments to answer these questions, although that seems somewhat unlikely. Experimental results seem to always give

larger straggle than predicted theoretically. Definitive theory would also be nice to have, but even before these two things are realized, perhaps there could be some sort of prescription which would allow the available codes to be altered to provide better answers.

CHOYKE

The main idea here is just to show that a factor of two uncertainty in the straggle is something that the experimentalists have a real worry about because it can give you terrible wiggles, or a smooth curve. And that makes a big difference.

MOFF

Here is a table (Table I-III) which shows calculated values of R_p and ΔR_p for 1 MeV He incident on stainless steel, as compiled by Choyke. The first two entries were calculated with EDEP using for a) the stopping powers values tabulated by Ziegler, and for b) the values of Northcliffe and Schilling. The last entry is from Brice's book. It is clear from the last column in the table that there is a range of ΔR_p values of a factor of two.

As a further indication of problems in the calculations Table I-IV shows some typical output from EDEP for He on 304 stainless steel using the Ziegler Chu stopping power. The important thing to note here is that the arrows indicate a range of energies for which the calculated straggle actually decreases with increasing energy. This is something which is clearly not correct, and it must indicate some numerical problems within the code.

CHOYKE

We have seen that happen in a number of cases, and for an experimenter it is quite worrisome.

ROBINSON

But it is known that there are numerical problems with the EDEP code. You can make changes in EDEP which move the problems around. Dean Oen has looked into this in some detail.

MORE

This figure (Figure I-3) now is, perhaps, the most scandalous of all. It may not really present a paradox, but the differences shown here are important.

CHOYKE

I don't think it is a question of paradox, but it is something which worries you. Suppose that you didn't know anything at all and you just naively plugged the Northcliffe and Schilling stopping powers into the EDEP code and you get these results which are so different from the other curves shown there.

MORE

These curves show the damage energy deposition distribution, $S_D(x)$, as calculated by EDEP in two cases, and from the Brice book in the other case, for 200 keV He incident on Zr. The curves labeled Z and N+S were calculated by EDEP using the Ziegler-Chu and Northcliffe and Schilling stopping powers respectively. These two calculations clearly give quite different results. The value in between is Brice's value.

CHOYKE

But actually Brice uses the Ziegler-Chu stopping.

BRICE

That's right. I used the Ziegler-Chu stopping in my calculations so that a comparison of my results with the curve labeled Z there represents a real difference in the codes.

MORE

That's not a difference in the energy partition function is it?

BRICE

I think that we both use the Lindhard energy partition function, so that part of the codes is essentially identical.

MORE

But that function is not really for either of these stopping powers but for the Lindhard stopping power, isn't it?

BRICE

That's right, but the energy partition function just applies to the recoils, so that the Lindhard function is probably quite adequate. The primary partitioning seen here in this figure though probably is dominated by the nuclear and electronic losses of the helium ion. As a further comment, I'd also like to point out that for light projectiles at low energies the Northcliffe and Schilling stopping powers are often in error by a large factor.

MORE

It may be that there is a lot of danger in the EDEP code in changing the stopping power in some parts of the code and not being consistent throughout. But, the question is, "What are we going to do about it?"

MUELLER

EDLP-1 has some problems which are intrinsic to it. It's a mistake to be using it as a standard.

MOPE

Except that it's readily available, and easy to use. And furthermore, if you wait for the ideal code to be written that will be years from now. And it may not happen. So we have to live with codes which are not perfect and see what we can do to live in the real world.

CHOYKE

An enormous amount of simulation work is being done which is based on computer codes. Mostly it's being done by users who don't have any idea what these codes do. And it's hoped that something will come from this meeting to improve that.

ROBINSON

Sounds like we should recommend that some source of funding be utilized in order to seek improvements in these codes. That is, until now everyone has depended on more or less DOE funded people to provide the tools of the trade, and since a large fraction of the implanters are now being used by private industry it might be that someone like IBM or Texas Instruments or some other corporation could be persuaded to fund such a project themselves. It is clear that improvements can be made. In principle, for example, it is possible to use the ACCUTRAN FORTRAN codes intended to transport neutrons and protons to transport atomic particles. We have been working on them for some period attempting to use ANISN in particular. ANISN is probably not good for ranges because it's

a one-dimensional code. It's great to use for sputtering calculations though. There are still some problems, however, associated with the optimum way of defining energy group structures. This occurs because the atomic particles slow down in a way which is different from the way in which neutrons slow down. These problems display themselves, at the moment, in values for the straggling which are much too large.

HAGGMARK

How about the forward peaked cross section?

ROBINSON

We handle that by going to a fairly high order Legendre expansion, P_0 , and then by cutting off and throwing away part of the electronic loss in a consistent manner. And basically the scattering cross section used is the Winterbon, Sigmund, Sanders version of the Lindhard cross section. We can improve things by going to potential scattering. Whether this whole approach will be a cost-effective approach or not we don't as yet know. It may be that TRIM, or something like that, will be more economical.

It seems to me that there are two separate questions which we are trying to address here. One is the calculational method and the other is the values of the parameters which go into the calculations. It's clear that if you ask the theorists to pick out, say for example, the electronic stopping law then only in accidental cases will it be proportional to the velocity and with the Lindhard coefficient in front. If you get that, lovely, but so what? You can cite example after example in the literature where the slope

ROBINSON

Also, one could take what experiment has wrought and then sort of back your way out of the calculation, according to some assumed law, to obtain the values of the parameters which best describe the basic equations. This could be done for a variety of cases, and then if things are consistent you have some confidence in the results. I don't think it's fair though to blame the theorists for a dispersion in calculated results which are due to the use of different starting data, or assumptions about the stopping law. Users of the various codes who put in their own values for these parameters, well, that's their own responsibility. On the other hand, the theorists do have some responsibility to take into account the experimental measurements which are available.

BRICE

Well, in light of the suggestion that we need to reach some sort of consensus relating to future work, one of the things which the theorists need to do is to state specifically what types of assumptions have gone into their work. Perhaps there needs to be a list appended to their work which says, for example, that a particular stopping law, or scattering law, etc., has been used in the calculations. In Zieglers book, for example, he doesn't mention where the straggle values come from.

ROBINSON

Is that possibly because the first volume of that set hasn't come out?

BRICE

Perhaps that is it.

TABLE I-1. RANGE, STRAGGLE CALCULATIONS

TABLE I-II. HELIUM IONS IN SOLID GERMANIUM (ENERGY - 1 MeV)

<u>METHOD</u>	<u>R_p (μm)</u>	<u>ΔR_p (μm)</u>
EDEP (LSS)	3.217	0.2556
JOGIBB (LSS)	3.2332	0.2526
MYLROIE BOOK	2.858	0.2503
EDEP (MYLROIE)	2.844	0.1818
EDEP (N&S)	2.935	0.1838
EDEP (BRICE)	3.091	0.2032
BRICE BOOK	3.089	0.2874

TABLE I-III. COMPARISON OF PROJECTED RANGE R_p (μm) AND THE
PROJECTED STANDARD DEVIATION ΔR_p (μm) FOR
1 MeV He IONS IN 304 SS

Method		R_p	ΔR_p
(a)	E-DEP-1 (Ziegler 1977)	1.647	0.0903
(b)	E-DEP-1 (Northcliffe and Schilling, 1970)	1.791	0.1231
(c)	Brice (1975)	1.821	0.1738

Ag on 304H (Ziegler & Chu)

$E(\text{MeV})$ $R_p(\mu\text{m})$ $\Delta R_p(\mu\text{m})$ $R(\mu\text{m})$ $\Delta R(\mu\text{m})$

2.400	3.807116	1.05993	3.807116	1.05993
2.450	3.848062	1.07281	3.848062	1.07281
2.500	3.900082	1.07985	3.900082	1.07985
2.550	4.003177	1.08465	4.003177	1.08465
2.600	4.173339	1.09410	4.173339	1.09410
2.650	4.272586	1.09792	4.272586	1.09792
2.700	4.368927	1.09725	4.368927	1.09725
2.750	4.463345	1.11093	4.463345	1.11093
2.800	4.564475	1.11720	4.564475	1.11720
2.850	4.664515	1.12253	4.664515	1.12253
2.900	4.765204	1.12505	4.765204	1.12505
2.950	4.867151	1.13786	4.867151	1.13786
3.000	4.970179	1.15457	4.970179	1.15457
3.050	5.074354	1.16471	5.074354	1.16471
3.100	5.179643	1.18584	5.179643	1.18584
3.150	5.286076	1.19267	5.286076	1.19267
3.200	5.393645	1.21013	5.393645	1.21013
3.250	5.502260	1.22093	5.502260	1.22093
3.300	5.612259	1.23260	5.612259	1.23260
3.350	5.723285	1.25601	5.723285	1.25601
3.400	5.835466	1.28393	5.835466	1.28393
3.450	5.948409	1.29274	5.948409	1.29274
3.500	6.063335	1.29644	6.063335	1.29644
3.550	6.179924	1.31290	6.179924	1.31290
3.600	6.295892	1.32397	6.295892	1.32397
3.650	6.413918	1.34113	6.413918	1.34113
3.700	6.533116	1.36850	6.533116	1.36850
3.750	6.653538	1.38364	6.653538	1.38364
3.800	6.775172	1.38364	6.775172	1.38364
3.850	6.898074	1.36455	6.898074	1.36455
3.900	7.022029	1.33191	7.022029	1.33191
3.950	7.147270	1.30430	7.147270	1.30430
4.000	7.273668	1.29447	7.273668	1.29447
4.050	7.401254	1.28391	7.401254	1.28391
4.100	7.530063	1.26232	7.530063	1.26232
4.150	7.660094	1.24729	7.660094	1.24729
4.200	7.791305	1.22440	7.791305	1.22440
4.250	7.923729	1.20477	7.923729	1.20477
4.300	8.057369	1.17491	8.057369	1.17491
4.350	8.192243	1.140757	8.192243	1.140757
4.400	8.328426	1.10057	8.328426	1.10057
4.450	8.465580	1.07231	8.465580	1.07231
4.500	8.603682	1.04711	8.603682	1.04711
4.550	8.742701	1.02496	8.742701	1.02496
4.600	8.882696	1.00486	8.882696	1.00486
4.650	9.023627	0.98681	9.023627	0.98681
4.700	9.165554	0.97079	9.165554	0.97079
4.750	9.308537	0.95681	9.308537	0.95681
4.800	9.452636	0.94386	9.452636	0.94386
4.850	9.597811	0.93193	9.597811	0.93193
4.900	9.744122	0.92099	9.744122	0.92099
4.950	9.891629	0.91001	9.891629	0.91001
5.000	10.040292	0.90000	10.040292	0.90000
5.050	10.190171	0.89096	10.190171	0.89096
5.100	10.341226	0.88287	10.341226	0.88287
5.150	10.493427	0.87572	10.493427	0.87572
5.200	10.646744	0.86951	10.646744	0.86951
5.250	10.801247	0.86424	10.801247	0.86424
5.300	10.956906	0.85990	10.956906	0.85990
5.350	11.113701	0.85648	11.113701	0.85648
5.400	11.271602	0.85398	11.271602	0.85398
5.450	11.430589	0.85240	11.430589	0.85240
5.500	11.590642	0.85174	11.590642	0.85174
5.550	11.751741	0.85200	11.751741	0.85200
5.600	11.913866	0.85318	11.913866	0.85318
5.650	12.077007	0.85528	12.077007	0.85528
5.700	12.241154	0.85830	12.241154	0.85830
5.750	12.406307	0.86224	12.406307	0.86224
5.800	12.572456	0.86710	12.572456	0.86710
5.850	12.739591	0.87287	12.739591	0.87287
5.900	12.907702	0.87954	12.907702	0.87954
5.950	13.076779	0.88711	13.076779	0.88711
6.000	13.246812	0.89558	13.246812	0.89558
6.050	13.417791	0.90495	13.417791	0.90495
6.100	13.589706	0.91522	13.589706	0.91522
6.150	13.762547	0.92639	13.762547	0.92639
6.200	13.936304	0.93846	13.936304	0.93846
6.250	14.110967	0.95143	14.110967	0.95143
6.300	14.286526	0.96530	14.286526	0.96530
6.350	14.462981	0.98007	14.462981	0.98007
6.400	14.640332	0.99574	14.640332	0.99574
6.450	14.818579	1.01231	14.818579	1.01231
6.500	15.000000	1.02978	15.000000	1.02978

MORE Figure I-1

MORE

Figures 1-2 a-c

MONTE Figure I-3

-- $S_D(x)$ for 200 keV He on Zr.

SOME LIMITATIONS IN THE SOLUTIONS OF RANGE/ENERGY TRANSPORT EQUATIONS

D. K. Brice

My contribution will be to review some of the main approximations and limitations which are commonly employed in calculations of the range and energy deposition distribution parameters through the use of the method of transport equations. These methods are the basis for many of the computer codes which are currently in use, and the problems associated with them are something that we all have to live with. Eq. (II-1) is a typical and more or less general transport equation governing energy deposition through the function $F(r, v)$, a distribution in spatial position r which depends on the projectile initial velocity, v .

$$-\frac{1}{v} \left| v \cdot \text{grad}_r F(\vec{r}, \vec{v}) \right| = N \int d\sigma_{n,e}(\vec{v}, \vec{v}', |\vec{v}_{e1}|) \left[F(\vec{r}, \vec{v}) - F(\vec{r}, \vec{v}') - F_h(\vec{r}, \vec{v}'') - \sum_i F_e(\vec{r}, \vec{v}_{ei}) \right]. \quad \text{II-1}$$

In this equation $d\sigma_{n,e}(\vec{v}, \vec{v}', |\vec{v}_{e1}|)$ is the differential scattering cross section for the projectile to change velocity from $\vec{v}$ to $\vec{v}'$ while simultaneously producing a target atom recoil with velocity $\vec{v}''$ and a number of excited electrons with velocities $|\vec{v}_{e1}|$. F_h represents the function F when the incident projectile is a target (host) atom, and F_e represents the function F for an incident electron. Equations similar to (II-1) govern both F_h and F_e , and these equations must be solved for F_h and F_e before Eq. (II-1) can be solved. A similar equation governs range distributions, however, F_h and F_e do not appear in that case.

In writing Eq. (II-1) a number of approximations have already been made. The most important of these are that it has been assumed that the target can be treated as if it were amorphous, that the interactions between projectile and target atoms and electrons are binary (or at least that the atomic collisions can be treated as binary), and that there are no important effects on F which can be attributed to the existence of a target surface.

Winterbon has altered the transport equations to include the effects of a target surface, but this involves including a cross section, $d\sigma_{n,e}$ which depends on r . This sort of change in the equation multiplies considerably the difficulties which arise in trying to obtain solutions; however, Winterbon has published some results for the altered equations.

MORE

Can you say how sensitive, in general, the calculations are to the approximation which neglects the surface?

PRICE

It varies, and it depends on whether you are dealing with an energetic ion which penetrates quite deeply into the target, or whether it has a small energy and only penetrates a few atomic layers. In the latter case the surface approximation is quite bad. Also, for sputtering calculations, i.e., for energy deposition distributions near the target surface, some sort of correction is required which is usually a large fraction of the calculated energy deposition at the surface. It is not clear how accurate these corrections actually are.

Now, another tacit assumption which has gone into writing the transport equation in this form is that charge changing collisions by the projectile can be neglected. I will point out the importance of this approximation presently, but first let me indicate further changes which are typically made to Eq. (II-1).

Several approximations are typically used to further simplify the transport equations. These include the assumption of the separability of the electronic and elastic energy losses, or more precisely that

$$d\sigma_{n,e} = d\sigma_n + d\sigma_e. \quad (\text{II-2})$$

Further, it is normally assumed that there is no straggle in the electronic energy loss, and that the electronic losses are individually small and do not lead to significant scattering of the projectile from a rectilinear path. With these added assumptions Eq. (II-1) becomes

$$- \frac{1}{v} \left| \hat{v} \cdot \text{grad}_r F(\vec{r}, \hat{v}) \right| - \frac{N S(E)}{2E} \left| \hat{v} \cdot \text{grad}_v F(\vec{r}, \hat{v}) \right| = \\ N \int d\sigma_n \left\{ F(\vec{r}, \hat{v}) - F(\vec{r}, \hat{v}') - F_h(\vec{r}, \hat{v}'') \right\} \quad (\text{II-3})$$

Here E is the energy of the projectile and $S(E)$ is the electronic stopping cross section for the projectile.

With this form of the equation it is also easier to see the importance of the charge changing collisions, which are generally neglected by everyone who does ion implantation calculations. The most important effect of these collisions is to alter the electronic stopping power $S(E)$. That is, the electronic stopping

power is not a unique function of E , but there are several functions, one for each charge state of the projectile. Thus, the term involving $S(E)$ should involve a sum over the various charge states, multiplied by the probability that a given charge state is occupied. These occupation probabilities, i.e., charge state fractions, will also be functions of energy. Thus, there will be an additional contribution to the straggle because of this effect. Winterbon has recently published a short paper on this, and he indeed finds that there is a significant increase in the straggle for the heavy ions because of these charge changing collisions.

ROBINSON

Can I point out that this may also influence the elastic scattering? At least it is something that ought to be looked into since you have particles with different screening involved in the collisions. In fact, you would have a distribution of interaction potentials as well.

BRICE

That's right, and none of the transport approaches to these calculations take these effects into account.

ROBINSON

Nor do anybody's calculations account for them as far as I am aware.

MORE

How much is that going to contribute?

BRICE

I haven't yet read Winterbon's paper carefully, but there are significant contributions from this effect. In a private

conversation with him he indicated that he thought that this might account for the 50% differences which are commonly observed between experimental and calculated range distributions.

Now, Eq. (II-3) is for an amorphous target, and although it appears that one is dealing with six variables, i.e., three each for $\vec{r}$, and $\vec{v}$, in practice one can reduce the number of variables to three. That is, $F(\vec{r}, \vec{v}) \rightarrow F(r, E, \eta)$ where $\eta = \vec{r} \cdot \vec{v} / rv = \cos(\vec{r}, \vec{v})$. Solutions to the equations are then typically obtained by going to a moments expansion of $F(r, E, \eta)$. Thus, defining $F_\ell(r, E)$ through

$$F(r, E, \eta) = \sum_{\ell=0}^{\infty} (2\ell + 1) F_\ell(r, E) P_\ell(\eta) \quad (\text{II-4})$$

and $F_\ell^n(E)$ through

$$F_\ell^n(E) = 4\pi \int_0^\infty r^{2+n} F_\ell(r, E) dr \quad , \quad (\text{II-4b})$$

one can convert Eq. (II-3) into an infinite set of coupled equations for the $F_\ell^n(E)$. The resultant equations are

$$\left\{ (n + \ell + 1) F_{\ell-1}^{n-1}(E) + (\ell + 1)(n - \ell) F_{\ell+1}^{n-1}(E) \right\} / (2\ell + 1) =$$

$$NS(E) \frac{dF_\ell^n(E)}{dE} + N \int d\sigma_n \left\{ F_\ell^n(E) - P_\ell(\eta') F_\ell^n(E - T) \right. \quad (\text{II-5})$$

$$\left. - P_\ell(\eta'') F_{h\ell}^n(T) \right\} ,$$

where T is the energy of the target atom recoil η' is the direction cosine of v' and η'' is the direction cosine of v'' . For these equations $\ell \leq n$ and is of the same parity. The boundary conditions

determine the type of distribution which the solutions describe. For a damage energy distribution one requires that $F_O^O(E) \rightarrow E$ at low energies, and for energy deposition into electronic excitation $F_O^O(E) \rightarrow 0$ at low energies. For range distribution F_h does not appear in the equations and $F_O^O(E) = 1$.

The Legendre coefficients are then the quantities which are usually solved for and they are related to the various moments of the distributions. The problem with trying to find the distributions by this method is that first of all there are an infinite set of equations to be solved. Then, notice that the equations are coupled through the left-hand term. That is, solutions to the n 'th order equation are required as source terms for the $n + 1$ st order equations. Since the equations must in general be solved numerically errors accrue in a given order solution which are then propagated into the higher order solutions. Further, since the moments are all taken about the origin, and not about the center of the distribution, the solutions are in general large numbers, and the central moments can be obtained only by taking the differences between large numbers. And, as an added feature the higher order equations require more calculational effort to obtain the same degree of accuracy as the lower order equations. The net result is that there is a practical upper limit to the number of moments which can be calculated, and thus a limit to the accuracy with which the distribution can be obtained. Usually only the first two moments are calculated for range distributions, although the tables of Johnson, Gibbons, and Mylroie have the

third moments, or skewness, tabulated. Also, Winterbon has given a method for obtaining accurate solutions for the higher order moments at low energies where the electronic contribution to the stopping power can be written as proportional to E^p with $p = 0.5$. His tables contain up to the fourth central moments for the range and energy distributions.

Table II-I lists some of the better known calculations of the moments of the projected range distribution, along with some limitations to the results. Similar data is shown in Table II-II for energy deposition distributions.

MORE

When you solve these equations you normally expand the integrand in T and convert the integral equation into a differential equation. You can do that because T is statistically a small quantity. Is the moments expansion itself an expansion in a small quantity?

PRICE

The energy T given to the recoils is on the average small relative to E because of the cross section. The moments expansion is, however, not an expansion in a small quantity. In this respect, as one goes to higher moments the higher energy transfers become more important, and ultimately, of course they dominate the highest moments. This is why the higher order moments require extra calculational effort. One of the difficulties in this method is then reconstructing the distributions after you have obtained the moments.

MORE

And the scattering cross sections are not necessarily very realistic.

BRICE

They are not realistic for the higher moments. In the tables indicating the calculation of the energy deposition distributions there are two different methods listed. The moments method is just a straight-forward reconstruction of the distribution from the moments as calculated from equations such as Eq. (11-5). The direct method has been used by a number of people, and it basically utilizes the fact that the range distributions can be represented by a small number of spatial moments, usually just two, and then the energy deposition distribution proceeds from knowing the projectile distribution at all energies as they slow to a stop. Most of the codes then neglect further energy redistribution by the recoiling target atoms, however, my code includes these recoil effects in the approximation of small recoil energies, which is usually the case. When the recoil effects are included in such direct methods the presence of the surface is partially taken into account in that recoils are allowed to carry energy away from the surface region, and there are no recoils to bring energy into the surface region.

This basically then summarizes the most important limitations to the application of transport theory to the calculation of the range and energy deposition distribution and, more or less, reviews the most common procedures for extracting the important information.

ROBINSON

Some of these limitations can be circumvented at some cost. The inclusion of OP_u and $2ER_{gce}$ and the avoidance of the moments method can be achieved through the use of the reactor codes I mentioned earlier. This approach would be best for the lighter ions since the codes were developed for neutrons and photons. For example, for sputtering calculations for light ions where Peter Sigmund's theory breaks down because the surface is more than just a perturbation it is possible to use ANISN to get excellent agreement with experimental data. The technique is quite powerful without having too much of a time limitation. At the present time there are some problems which seem to be associated with selecting the appropriate energy groupings for carrying out the basic integrations over the cross section at various stages in the calculation. It is not clear, however, that this will ultimately be a better approach, and it may be that we will have to abandon transport theory altogether in favor of atomistic methods which, whatever other approximations may be used, can be made fast enough to accomplish the calculations as, for example, TRIM does. I haven't actually used TRIM, but for some applications it seems to be a reasonably fast code.

HAGGMARK

Well, it's like any other Monte Carlo or simulation calculation. You have to run a number of particles, a number of histories. The time limitations depend on the energy of the particle, and how finely you want to know the details. If you just want the first

and second moment you don't always get a good representation of the distributions since they seem to be skewed. So you want to get the third and fourth moments. Biersack has been using TRIM to get these moments, but you run into the same problems that you find in the transport calculations, that these moments require extra time on the computer. You are out in the wings of the distributions for these moments, and there are usually not many particles out there, in the Monte Carlo sense, so you are going to have large uncertainties.

ROBINSON

But you can also evaluate the distribution function directly, and you know the statistics, and can assess the accuracy right away. In general, you have adequate control so that this may be a more cost-effective way to get the answers. Part of the attractiveness of transport theory, in my opinion, derives from the early days of reactor physics when everyone tried to use Monte Carlo techniques. The computers then were not capable of handling the problems associated with Monte Carlo, they just weren't fast enough and didn't allow elaborate enough models to be built, so that the reactor people built up this big body of transport theory. In recent years there has been a tendency to go back to the Monte Carlo methods, however.

MORE

Isn't that just because neutron problems can be described just by multi-group diffusion?

ROBINSON

Yes, that's just transport theory.

MORE

But it doesn't have the angular resolution.

ROBINSON

You don't really need the angular detail, but there is nothing to prevent you from getting it. In fact in some cases, for photon transport, one has to take into account anisotropic scattering.

ROBINSON

In fact, codes like MORSE and ANISN are designed not only for reactor applications but also for a wide range of applications, such as, for example, calculating the shielding of a space vehicle of more or less complicated geometry.

MORE

But isn't it true that in order to get the angular resolution one needs to go to relatively high order Legendre terms?

ROBINSON

It has been necessary in our sputtering calculations to go to P_9 terms, which in reactor terms is very high order, they typically use P_2 . But, you can do it. The codes allow for it. It is relatively slow. I think however that the Direct Monte Carlo codes are quite useful. It allows for the surface, you get the distribution function directly, you can include any electronic stopping law, it isn't limited to velocity proportionality. It handles potential scattering directly without any fiddling around; you need the transport cross section for transport theory calculations. It just has a number of advantages.

BRICE

What are the problems associated with going to high energies in the Monte Carlo calculations?

HAGGMARK

Well, Biersack came up with this path-length stretching, I'm not going to go into it in detail, but it's a way of stretching the distance between collisions by using some average properties of the projectiles over a long distance. Then we pick the closest collision, in a random sense, which will happen over that path length. The only restriction made in our code in this stretching is that the electronic energy loss not exceed about 5% over the path length, so we don't just wipe out the problem. It seems to give good results when we compare the atom-by-atom collision calculations with those using path-length stretching, and it does save a lot of computer time.

TABLE II-I. RANGE DISTRIBUTION SOLUTIONS

I. NUMERICAL

- a. First Order Expansion of Integrand
(Mueller & Manning, Gibbons & Johnson,
range and straggle only).
- b. Second Order Expansion
(Brice, range and straggle only).
- c. Higher Order Expansion
(Gibbons, Johnson & Mylroie; range, straggle,
and skewness).
- d. Low Energy, Infinite Order Expansion
(Sigmund, Matthies & Phillips; range and
straggle only).

II. ALGEBRAIC

- a. Low Energy, Infinite Order Expansion
(Winterbon; through fifth moments).

TABLE II-II. ENERGY DEPOSITION DISTRIBUTIONS

I. DIRECT

- a. Mueller & Manning - EDEP-1
(neglects energy transport by recoils).
- b. Brice
(includes recoil energy transport).

II. MOMENTS (LOW ENERGY)

- a. Numerical - Sigmund, Matthies & Phillips
(only through second moments). $M_1 = M_2$
- b. Algebraic - Winterbon
(through fifth moments).

THE EFFECT OF THE SCATTERING CROSS SECTION ON STRAGGLE

G. Mueller

The work that I am going to report will not be a definitive examination of the dependence of straggle on the scattering cross section used in the calculations, but I will talk about some of the effects which can be expected. I did some model calculations in which I varied the elastic scattering potential. To parameterize the various potential functions I used a Moliere potential for r less than some value r_c and a Born-Mayer type of potential for r greater than r_c . Thus

$$V(r) = \begin{cases} V_{\text{Moliere}}(r) & , r < r_c \\ V_{\text{BM}} e^{-\beta_{\text{BM}} r} & , r > r_c \end{cases} \quad (\text{III-1})$$

The two regions were joined by requiring that the value and slope of the two functions be equal at $r = r_c$. This leads to a family of potential energy curves, each characterized by a value of r_c , as indicated in Figure III-1. This figure shows the curves obtained for a copper-copper interaction. The solid curve is the Thomas-Fermi potential, the large dashed curves are the Moliere potential with screening length $a = 0.15 \text{ \AA}$ for the upper one and $a = 0.0738 \text{ \AA}$ for the lower. The larger screening length gives a potential which is close to the Thomas-Fermi potential, while the smaller screening length is one recommended by Torrens and Robinson. All the short dashed curves are the potentials of Eq. (III-1) using the upper Moliere curve with the matching prescription just described.

Figure III-2 shows the relationship between the elastic energy transfer, T , and the impact parameter squared, p^2 , for 10.5 keV Cu incident on Cu using the potentials described in Figure III-1. For the smaller values of r_c you can see that only the small values of the impact parameter give any appreciable energy transfer, and thus by varying r_c one is effectively varying the distribution of energy losses.

I have used the MARLOWE code along with the family of potentials just described to investigate the effects of varying r_c on the mean range and the straggle for 10 keV Cu incident on Cu. The results of these calculations are shown in Figure III-3. Plotted there are mean range and straggle versus r_c . The X's are the mean range; the circles are the straggle values. At large values of r_c the variation in both these quantities is relatively flat and approximately what one would expect from the Thomas-Fermi potential since we are in effect just using the upper Moliere potential in Fig. III-1 for most collisions. At lower values of r_c , however, one sees a strong dependence of both range and straggle on r_c . The values shown with the lines drawn through them are just the results obtained by doing the same calculation using the Torrens and Robinson version of the Moliere potential.

ROBINSON

George, let me ask a couple of specialized questions. What cutoff in impact parameters did you use in MARLOWE? And, did you use an isotropic source in a single crystal target?

MUELLER

I used 0.51 for the impact parameter cutoff, and yes, I used an isotropic source in a single crystal target.

SPITZNAGEL

The range apparently goes up because you are effectively reducing the number of collisions at small r_c . Why does the straggle go up?

MUELLER

The collisions which remain are essentially high energy loss collisions.

MORE

And they are relatively large angle collisions since you have dropped that part of the potential which leads to small angle collisions.

ROBINSON

Which range is this, George? Is this the automatically reported range from MARLOWE, or some other range?

MUELLER

This is the projected range. The importance of the data in Fig. III-3 is just to show that the choice of scattering potential can have a relatively large effect on the calculated straggle.

PARKIN

Is there some sort of general conclusion you want to make concerning these figures?

MUELLER

Basically, I wanted to show that the straggle depends quite sensitively on the scattering potential used in calculations of this

type. You can see also that in addition to that, the ratio of the straggle to the range also changes considerably. So that in essence the shape of the distribution is sensitive to the scattering potential. I guess that the main conclusion is that the calculations ought to use the best possible potentials and cross sections.

In order to extend these calculations to higher energies I have used a somewhat different procedure. Namely, I have parameterized the elastic scattering cross section, and then by reversing the procedure I obtain a potential corresponding to a given cross section. The parameterization technique that I use is based roughly on the form which Winterbon has used for the Thomas-Fermi scattering cross section. That is,

$$d\sigma = \pi a^2 f(\eta) \eta^{-2} d\eta \quad (\text{III-2})$$

where a is the screening length and $\epsilon = (T/T_m)^{1/2}$. Here T is the energy transfer, T_m is the maximum energy transfer and ϵ is the projectile energy in the reduced units of Lindhard. Winterbon gives $f(\eta)$ for Lindhard's Thomas-Fermi cross section as f_W , where

$$f_W(\eta) = \lambda \eta^{1/3} [1 + (2\lambda)^{2/3} \lambda^{2/3} \eta^{8/9}]^{-3/2} \quad (\text{III-3})$$

with $\lambda = 1.309$. For my own parameterization I choose a two branch representation of f ,

$$\begin{aligned} f_{nm}(\eta) &= g_u(\eta) , \quad \eta > \eta^* \\ &= g_{nm}(\eta) , \quad \eta < \eta^* \end{aligned} \quad (\text{III-4})$$

and

$$g_u(\eta) = \frac{a + 0.5\eta}{b + c\eta + \eta^2} \quad (\text{III-5a})$$

$$g_{nm}(\eta) = \frac{A\eta^{nm/4}}{[B + \eta^{m/4}]^n}$$

With an appropriate choice of a , b , and c , the upper branch reproduces Thomas-Fermi to within a few percent, while the lower branch is adjustable with essentially three parameters. After matching slope and value at $\eta = \eta^*$, the three parameters are n , m , and the value of η^* . This gives you an enormous flexibility in choosing scattering potentials. You can turn the LNS procedure around now and find a potential function for each choice of the various adjustable parameters to obtain a family of potential curves. Then you take a phenomenological potential for which you need the scattering cross section, and by matching the family of potentials obtain the member which best represents the chosen potential and the scattering cross section is then given by the appropriate f_{nm} . Figure III-4 shows several potential functions compared with one member of this family. The solid curve is a Genthon potential, the two Moliere potentials are for the Torrens and Robinson screening length (lower) and the Firsov screening length (upper) while the uppermost potential is the Lindhard Thomas-Fermi potential. One of the family members of my set of potential functions is shown as the small dashed line, and the parameters have been chosen so that the Genthon potential is well matched, at least down to very low energies.

ROBINSON

I would just like to comment that you should be careful how you reference these various potentials and cross sections with regard to the Thomas-Fermi model. You can, for example, take the Winterbon, Sigmund, and S. nders Thomas-Fermi cross section and perform the Firsov inversion procedure to obtain the potential, and what you get is not really a potential at all, since it depends on the projectile energy. But in any case, the result more nearly approximates the Moliere potential, rather than the Thomas-Fermi potential, that is it falls off more rapidly than the Thomas-Fermi potential. Probably the WSS scattering law should not be referred to as the Thomas-Fermi scattering cross section, although it has some relation to the Thomas-Fermi potential, but then so does the Moliere potential.

MUELLER

That's right. It's really the Lindhard approximation to the potential. What I did is start with a pair of approximations, the LMS approximations, which will take you from exact scattering theory to the Lindhard cross section. There is an inversion of this process which will take you from the Lindhard approximation of the cross section back to the real potential.

Well, what I did was just take this scattering cross section, i.e., the (2,3,0.02) family member, and compare range and straggle calculations made with it and with the Lindhard approximation to the Thomas-Fermi scattering cross section. These results are shown in Figure III-5 where range and straggling are plotted as a function of energy for Cu incident on Cu. Note that there is

no difference in the two types of calculation for energies above about 100 keV, but below that energy there is considerable difference both in the absolute values, and in the ratio of straggling to range. This is just for Cu on Cu, of course, but it turns out that in general when $E/E_L < 0.1$ then it is probably a good idea to use some better approximation to the cross section than the usual Lindhard version of the Thomas-Fermi cross section.

ROBINSON

But you can only judge that on the basis of some experiment which measures some of these quantities in the appropriate energy range. That is, how will you determine that one potential is better than another?

MUELLER

Well, if you are interested in a low energy then the Lindhard approximation to the Moliere potential does much better than the Lindhard approximation to the Thomas-Fermi potential.

ROBINSON

I should comment about that copper potential parameter of Torrens, and that is that John Schiffgens has put that into his dynamical code and used it to calculate the displacement threshold and he finds that it agrees well with experiment.

MUELLER

Well, in any case, it's clear that if you are going to do analytical transport theories of the Lindhard type it is very little more difficult to use a Moliere potential rather than the Lindhard approximation to the Thomas-Fermi potential, and it's better.

Now maybe I should say a few things about the code EDEP-1, since it has been mentioned prominently in regard to the range and straggle calculations. Basically, it should not be used as a standard. It uses the Johnson and Gibbons subroutine for calculating the straggle, and they say that this routine is not to be trusted. It's based on a first order expansion of the integral equations, and the ion-target combinations for which the results are unreliable depends on the machine you run the code on. Their new one, the one they did with Hydroie, apparently doesn't have this problem.

MORE

But the troubles with the earlier version must be a problem with the coding. That is, the new version may change the answers, but the incremental straggling should be positive as you increase the energy.

BRICE

Well, there seem to be some problems with the equations themselves at very low energies. That is, the solutions for the straggle turn out to be negative, and this may be associated with a lack of convergence of the expansion, or the fact that an insufficient number of terms are included in the expansion.

MUELLER

One last thing, we have been trying some new methods for solving the equations which avoids making the expansion of the integrand. We do it by a matrix method, and the solution then just depends on inverting a matrix. The calculation goes quite fast, and the slowest part is the inversion of the matrix.

MUELLER Figure III-1

MUELLER Figure III-2

MUELLER Figure III-3

MUELLER Figure III-4

MUELLER Figure III-5

MONTE CARLO CALCULATIONS OF RANGES AND STRAGGLINGS

L. G. Haggmark

I would like to begin my remarks by describing briefly for you some of the features of the TRIM code, including in particular the manner in which the electronic and nuclear energy loss is handled. Then, I'll present some sample calculations for comparison with experiment and other calculations, and finally, I will compare the results of the calculations with some recent experimental data for deuterium incident on C, Al, Ni, and Zr, and with their calculations of range and straggle.

The advantages of the calculations by Monte Carlo ion transport methods are that one can take explicit account of interfaces; it gives a rigorous treatment of nuclear scattering; and it provides an easy determination of the energy and angular distributions. The major limitation of this approach is that it is time consuming on the computer. This latter depends on just what type of detailed information is sought in the calculations.

SPITZNAGEL

Can you say something about the time limitations for those of us who don't have much big machine experience: Say, as compared with EDEP?

HAGGMARK

EDEP is a very fast code, and I'm sure that there you are talking about tens of seconds, while I'm talking here about minutes for low energies up to maybe a half hour for the higher energies on a machine like the CDC 6600 or 7600. Let me defer this question to my last

set of results where I do have some information on the exact times. I knew the question would come up, so that's why I prepared for it.

In the Monte Carlo approach we are, in general, following a large number of particle "histories". Each particle starts with a given energy, position, and direction of motion. We allow the particles to move in straight free-flight-paths between nuclear collisions, whereupon the particle changes its direction of motion. The energy is reduced by both nuclear and electronic energy losses, and the history is terminated when the particle leaves the target, or its energy drops below a predetermined minimum, typically 5 eV. In the TRIM code we apply these techniques to amorphous targets in the binary collision approximation. We use a fixed distance between collisions, which represents the average distance between target atoms, and the scattering angle and energy loss are randomly selected at each collision.

ROBINSON

Do you stick in a free flight distance between collisions to preserve density?

HAGGMARK

We just assume that there is a collision each time the projectile covers a distance of $N^{-1/3}$, where N is the atomic density, and we select our impact parameters from an area of size $N^{-2/3}$ at each collision. This preserves the correct atomic density.

In our treatment of the nuclear scattering and energy loss we are able to use realistic atomic potentials, and we represent the scattering event by an analytic formula. This latter gives us a very rapid assessment of the scattering angles and energy loss.

At low projectile energies ($\epsilon < 1$), the electronic energy loss is represented by S_L , with

$$S_L = k E^p \quad , \quad (IV-1)$$

where $dE/dx(\text{electronic}) = -N S_L$. As default values for k and p we use the Lindhard values, $k = k_L$ and $p = 0.5$. For hydrogen and helium isotopes we use the Anderson and Ziegler compilations. At high energies ($\epsilon > 10$) we use something close to the Bethe-Bloch formula to obtain S_H . And finally, at intermediate energies ($1 < \epsilon < 10$) we use a formula due to Biersack for S_I , namely

$$1/S_I = 1/S_L + 1/S_H \quad . \quad (IV-2)$$

In Figure (IV-1) we show the nuclear scattering event, and define the various quantities and symbols associated with the event. On the basis of this geometry Biersack has given an approximate, but fairly accurate analytical formula for treating the nuclear scattering. This is illustrated in Figure (IV-2) where the "scattering triangle" is shown. The basic approximation in the Biersack treatment is to take the quantities δ_1 to be small. Precisely one can write

$$\cos \frac{1}{2} \theta = \frac{P + \rho + b}{r_o + \rho} \quad (IV-3)$$

where P is the impact parameter, $\rho = \rho_1 + \rho_2$ with the ρ 's as defined in Figure (IV-2). From classical mechanics it is easy to show that

$$\rho = \frac{2[E_o - V(r_o)]}{-(dV/dr)_{r=r_o}} \quad . \quad (IV-4)$$

For the value of δ in (IV-3) we use a five parameter fitting formula which is based on the Rutherford scattering formula, and it is parameterized such that as the center of mass energy, E_c , becomes large δ approaches the result one would obtain from the Rutherford formula. The value of δ is obtained by a fit to precomputed scattering integral results and these functions are available for potentials of the form Thomas-Fermi-Sommerfeld, Moliere, Bohr, Lenz-Jensen, Wilson-Haggmark-Biersack, and the Kalbitzer-Oetzmann potential. Figure (IV-3) shows a comparison of our $\sin^2 \frac{1}{2} \theta$ as a function of P/a , where a is a screening length, with exact values as calculated by Robinson for the Moliere potential. You can see that there is essentially no difference on this logarithmic plot. The maximum differences are usually less than 1-2%. The ϵ -values on the plot are the projectile energies in Lindhard dimensionless units.

Figure (IV-4) shows similar results at higher energies, where we also compare with the results from the Rutherford formula. Once again the approximate formula is seen to reproduce quite well the results from exact calculations.

Figure (IV-5) shows a comparison of our calculations with TRIM using a Moliere potential with calculations by Brice using transport equation methods, and with experimental results from two different laboratories for boron incident on silicon. These results show that our calculations compare quite well with both the calculations of Brice, and the experiments over the energy range shown ($\epsilon \sim 4$ to $\epsilon \sim 20$).

Figure (IV-6) shows the actual depth distribution of implanted boron, incident on silicon at 100 keV, as obtained from TRIM

calculations and from the experimental results of Hofker, et al. Their distribution is slightly deeper than our calculated distribution, and also a little bit wider. We have not included electronic energy loss straggling in the calculations shown here, but even when we do put it in it is quite small, and we see essentially no effect. Probably the main discrepancy on the width here is in taking out the detector resolution on the experimental curve.

Figure (IV-7) shows similar results for ^3He incident on niobium at 150 keV. Again the calculations agree quite well with the experimental data when a value of k equal to 1.5 times the Lindhard value is used in the stopping power formula.

Figure (IV-8) shows further results for ^3He on niobium, but at a much lower energy. These results are compared with the experiments of Behrisch, et al. The experiments are very difficult at this energy, and it is probably fortuitous that the mean range in our calculation agrees so well with the mean range of the experimental data. The MARLOWE results shown are their calculations, which also seem in reasonable agreement with the predictions of TRIM.

Figure (IV-9) shows a comparison of the mean ranges calculated by TRIM and by MARLOWE, as a function of energy, for ^4He incident on copper. The agreement there is seen to be quite good, generally less than 10% difference, over the two orders of magnitude in projected range which are plotted.

Figure (IV-10) shows a comparison of some calculated distributions with the results of a round robin experiment in which SIMS measurements of the depth distribution of H implanted at 40 keV Si were made by a number of laboratories. The results of these

experiments which were organized by Jim Ziegler, are shown as the smooth solid curve. The dashed curve is the results of calculations by Brice's RASE3 code and the solid histogram is from the TRIM Monte Carlo calculations. For the TRIM calculations we used $k/k_L = 1.6$ which gave a mean penetration depth about equal to the experimental curve. I ran Dave's code with the same values of k to get the dashed curve. We get the same average depth, but I don't recall the exact value for the straggling in these two cases.

BRICE

The curve calculated from my code looks a little wider, but then you have some extra tail over there to the left.

HAGGMARK

Certainly for the FWHM yours is wider.

Now, I'd like to show some more recent work for deuterium incident on several target materials. Børgesen, Böttiger, and Møller at Aarhus implanted D into several targets and then used the ^3He nuclear reaction to obtain the depth profiles. I think that this was reported in Journal of Applied Physics last August. They reported values of the most probable range and the full width at half maximum for these measurements, and they also carried out some Monte Carlo calculations for comparison. The calculations used Anderson-Ziegler electronic stopping with the LSS form of the elastic scattering cross section.

Figures IV-11 through IV-14 show the results of the measurements and the calculations. It can be seen there that the most probable ranges are in good to fair agreement, while the FWHM values are

consistently underestimated by the calculations by 20-100%. This intrigued me and I decided to do the same calculations using the TRIM code. In general, we reproduce the most probable range calculations over the energy range shown, and we are in fair agreement with the FWHM calculations at the higher energies. This depends somewhat on the target material, but our calculation often deviates from the Aarhus calculations at the lower energies. Now, these experiments were carried out at, I believe 50 K, so that there should be no diffusion. Also, they subtracted experimental resolution from their data.

CHOYKE

What is their experimental accuracy in the FWHM?

HAGGMARK

They claim that it is about equal to the size of the points on my graphs. I picked their values off their plots and it was just not worthwhile putting the error bars on since they were about the size of the symbols.

BRICE

Which elastic scattering law did you use? The Lindhard version?

HAGGMARK

No, I used the Moliere. The Aarhus group used the LSS version.

BRICE

So the excess straggle is not due to the potential used then?

HAGGMARK

Yes, that's right.

Finally, let me present some results which I obtained by changing the screening length in the Moliere potential. I chose to do these calculations for 10 keV D incident on Ni and used $k/k_L = 1.08$. The results of these calculations are summarized in Table IV-I where the first column is the experimental results from the Aarhus group, the second column shows calculated results using the Firsov value for a , the third column is for an a -value $3/4$ ths of the Firsov value, and the fourth column is for an a -value 1.5 times the Firsov value. The quantities tabulated are mean range, FWHM, and the reflection coefficient, R_N . The experimental value for R_N is from Eckstein and Verbeek.

RRICE

It appears there that the ratio of FWHM to R_p doesn't change very much for the different values of a . From about 1.05 to 1.2 over the range of a -values you considered.

HAGGMARK

Yes, that's right.

Let me finally give you some times for the operation of the TRIM code on the CDC-7600 at Sandia Livermore. I ran 5, 10, 15,...up to 35 keV; I ran 5000 histories in each case with a free-flight distance of $N^{-1/3}$ and with a 5 eV cutoff. The 5 keV took 7 minutes, 10 took 11 minutes, and at 35 keV it took 25 minutes.

ROBINSON

It should go approximately logarithmically.

HAGGMARK

Right.

TABLE IV-I. COMPARISON OF R_p , FWHM AND REFLECTION COEFFICIENT R_N OBTAINED FROM EXPERIMENT WITH TRIM CALCULATIONS USING DIFFERENT SCREENING LENGTHS. $D \rightarrow Ni$, $E_0 = 10$ keV; MOLIERE POTENTIAL, $k/k_L = 1.08$.

	EXPERIMENT	TRIM		
		FIRSOV a	0.75 x FIRSOV a	1.5 x FIRSOV a
R_p (°)	875*	875	1000	750
FWHM (Å)	1310*	975	1050	900
R_N	0.085**	0.097	0.087	0.111

*Bjergesen, Böttiger, and Möller

**Eckstein and Verbeek

NUCLEAR SCATTERING

SCATTERING INTEGRAL (CLASSICAL MECHANICS)

$$\theta = \pi - 2 \int_{R_0}^{\infty} \frac{P \, dr}{r^2 \left[1 - V(r)/E_c - P^2/r^2 \right]^{1/2}}$$

R = INTERATOMIC SEPARATION

R_0 = DISTANCE-OF-CLOSEST APPROACH

P = IMPACT PARAMETER

$V(r)$ = INTERATOMIC POTENTIAL

E_c = CENTER OF MASS ENERGY

"SCATTERING TRIANGLE"

$$\rho = \rho_1 + \rho_2,$$

$$\delta = \delta_1 + \delta_2$$

$$\cos \frac{\theta}{2} = \frac{P + \rho + \delta}{\rho + R_0}$$

HAGGMARK Figure IV-2

HAGGMARK Figure IV-3

HAGGMARK Figure IV-4

HAGGMARK Figure IV-5

HAGGMARK Figure IV-6

HAGGMARK Figure IV-7

HAGGMARK Figure IV-8

HAGGMARK Figure IV-9

HAGGMARK Figure IV-10

HAGGMARK Figure IV-11

HAGGMARK Figure IV-12

HAGGMARK Figure IV-13

HAGGMARK Figure IV-14

DAMAGE STUDIES IN ALUMINUM

T. S. Noggle

We have used a thin film electrical resistivity specimen as a damage sensor to study the depth distribution of damage for a number of different atomic projectiles incident on aluminum. The specimen thickness, $0.38\text{ }\mu\text{m}$ for the measurements reported here, was small compared with the incident projectile ranges, which were selected to be about ten times the target thickness. The depth variation of the damage for the chosen projectiles was then studied by interposing various thicknesses of absorber foil between the beam and the target specimen. The resistivity specimen thus samples a distribution of projectile energies the same as that expected for a slice of target material at the given depth in a thick target.

The data will be presented as relative damage rates, not absolute damage rates. That is, the measured resistivity for a given thickness of intervening absorber foil is divided by the resistivity for the open beam measurement when no absorber foil was present. This is one way of eliminating some of the experimental uncertainties which plague the absolute measurements, such as the thin film effects in resistivity measurements, etc. Measurements have been made for Mg, Al, Si, P, S, Cl, and Ar ions incident on aluminum specimens with incident energies chosen such that the projectile range is about $3.5\text{ }\mu\text{m}$ for each case. This involves varying the incident energy from 4.6 MeV for the Mg ions up to 6.0 MeV for the Ar ions.

Figures V-1 through V-7 show the results of these experiments where the damage ratios are plotted as a function of the interposed absorber foil thickness. Also shown on these figures are damage energy deposition distributions calculated using the EDEP code where the electronic stopping constant k has been adjusted so that the experimental and theoretical curves are in agreement over the leading edge of the damage peak. We have somewhat more confidence in these experimental points as compared with, say, those on the backside of the curve since multiple scattering effects may be such that these points do not properly represent the corresponding portion of a thick target damage distribution.

From a consideration of the multiple scattering effects we should expect that the calculated and measured damage distributions would differ by no more than a few percent at the damage peak. We find typically, however, that the difference is of the order of 10-15%, with our measurements being lower. This deviation is perhaps not too bad considering the uncertainties which we have already discussed today concerning the EDEP code.

One of the things which we have done is to look for systematic deviations in various comparisons between experiment and theory as the ion mass is changed, and some of our results are summarized in Table V-I. There one can see that the peak to surface damage ratio decreases with increasing ion mass in both experimental and theoretical estimates, although the experimental values seem to drop somewhat more rapidly.

The last two columns of the table compare the total damage energy with the total damage as measured by the resistivity measurements,

with, in both cases the value for aluminum ions taken as a normalization constant. The two cases in which there is a large difference between the experimental and theoretical values represent cases in which the experimental uncertainty in the open beam resistivity was relatively large. In summarizing the data in the table I would say that EDEP does quite a good job for the heavy ion case.

Figure V-8 shows the values of the electronic stopping parameter k extracted from our comparisons between experiment and theory along with the values predicted by the Lindhard formula. The agreement between our values and those of Lindhard is close for the light ions in our studies, but our values are systematically higher for the heavier ions. This is a reflection of the well known oscillatory behavior of the electronic stopping power. I should interject that there is still some uncertainty in the precise values of the thickness of our absorber foils, so that the k -values plotted here may change by 5% or so as we refine our measurements. The relative values are, however, quite good since we use the same set of absorbers for each of the experiments reported here. We should report, however, that the k -value does seem to vary somewhat with energy. We have, for example, data for 2.7 MeV Al on Al for which the best fit to the damage curve gives a k -value of 0.138. This should be compared with the k -value of 0.143 determined from the 4.8 MeV measurements. Although these values are not too far apart we believe they represent a true variation of k with E .

One of the goals of our work is to carry out a normalization of ion to neutron damage. The general idea is that in the ion simulation work people use various codes to obtain the dpa resulting

from a given ion dose, and other codes are used to obtain similar data for neutrons. In view of the approximations involved in the theory, one doesn't really know how well the neutron damage can be compared with the ion damage, particularly because of the significantly different range of recoil energies in the ion case. One of the problems one encounters when attempting to do these comparisons is that there is considerable scatter, of the order of 20%, when one attempts to measure the damage for a fixed experimental case. Some results illustrating this are shown in Table V-II.

What we have done to get around the problem is to carry out experiments for both ions and neutrons incident on a given thin film specimen and for the neutrons incident on a bulk specimen irradiated along with the thin film specimen. Thus we have a direct normalization of thin film damage rates to bulk material damage rates for the neutrons and also the internal normalization of ion to neutron damage rates in the thin film specimen. Typical results of such comparisons are shown in Table V-III. The bottom line of the comparisons of this table is that the ion to neutron damage ratio for 4.8 MeV Al ions in Al as compared with a fission neutron spectrum is 2.35×10^4 . This is about 6-7% lower than the equivalent damage energy ratio and indicates very good agreement between experiment and theory, since the difference is less than the experimental uncertainty estimated to be about 10%. Measurements made of the damage rates of 300 keV protons and 1 Mev α -particles in Al, normalized to the 4.8 Mev Al damage rate, gave results that were about 50% lower than the equivalent ratios obtained from EDEP

using a value of 0 for the displacement threshold energy E_d . If the calculations are made for $E_d = 20-30$ eV, the agreement between experiment and theory is within the experimental uncertainty. The use of a 20 eV threshold value in the calculations for the self-ion and fast neutron case are shown in Table V-III and show even better agreement between the experimental ratio and the calculated ratio. This perhaps is gilding the lily, but it does indicate that a reasonable correction to the theory leads to better agreement rather than vice-versa. To sum up the results for Aluminum, we find that for the heavy ion case the agreement between experiment and theory (EDEP) is excellent over a large fraction of the range of the ions and differs by only 10-15% at the damage peak position. The normalization of self-ion to fast neutron damage leads to very good agreement between experiment and theory.

Finally, I would like to report that we have similar results for Ni targets, although there are some experimental problems which we do not as yet understand. The various results are reproducible, however, so we have at least demonstrated that we can reproduce what we don't understand. Figure V-9 shows typical results for 17.4 MeV Ni ions incident on Ni where we have plotted the absolute damage rate as measured by resistivity (since our experimental problems involve the interpretation of the open beam damage as a function of dose we have chosen not to normalize). The damage energy scale for the theoretical calculations was adjusted so that the experimental points are closely matched by the curves. The two calculations are from EDEP, with $k = 0.162$, a value close to the Lindhard value,

and from Brice's book where the Northcliffe-Schilling stopping powers were used.

BRICE

The foils in your experiments are always of the same type of material as the target.

NOGGLE

Yes, here we used nickel foils in front of the nickel target, although they were from a different source.

I think that we are going, ultimately, to find that Ni behaves pretty much like aluminum. We do, however, have yet to understand the open beam dose effects. The general level of agreement between theory and experiment suggests that we will probably be able to compare the ion and neutron damage in much the same way. That is, theory and experiment seem to scale well with ion energy, thus, I feel it will carry over to the neutron case.

For the lighter ions, hydrogen and helium, we find quite a different behavior for Al targets. The open beam damage rate, as predicted by EDEP, scales with the damage energy quite well, so we feel justified in normalizing the damage curves to the open beam damage. When we do this, however, we find that the experimental damage rates are a factor of two or so larger than the theoretical damage rates in the vicinity of the peak. We don't understand this but we speculate that there may be significant backscatter near the end of range which is not included in the EDEP calculation.

BRICE

I think that EDEP is probably much like my code in this respect and some of this backscattering is taken into account. That is, the

ion distribution is allowed to spread out appropriately in space so that the presence of backscattered particles is taken into account at each depth in the target. Both our codes, however, may not properly take into account the directionality of the backscattered (or more precisely, large angle scattered) component. That is, those particles scattered through large angles may spend a larger than average amount of time at a given depth and thus contribute proportionately more to the damage near the peak. So it is probably correct to say that while the codes take the backscattered particles into account they only do so in an approximate manner, and your comment about the source of the large differences observed for these lighter projectiles may indeed be correct.

What sort of dose do you have in these experiments, Tom? Could some of the damage be just apparent damage due to the implanted hydrogen itself contributing to the resistivity?

NOGGLE

I can't give you actual numbers for the total hydrogen stopped in the specimen because of the way we do the experiment. Much of the hydrogen passes on through the thin film specimen into the substrate. In the course of the experiment we have a total dose of about 10^{12} ions/cm², which represents the sum of the doses delivered in 20-30 discrete irradiations. Approximately 90% of the irradiation dose was obtained in open beam of thin absorber foil irradiation for which the vast majority of the ions would be stopped deep in the substrate.

BENEDEK

To decide whether the resistivity of the implanted ions is

significant, one must know the ratio of Frenkel pairs produced per incident ion to the fraction of incident ions that are stopped within the specimen. Under most circumstances the former is at least two orders of magnitude greater than the latter. Therefore, the resistivity of the implanted ions is negligible.

TABLE V-I. COMPARISON OF EXPERIMENT AND THEORY FOR HEAVY
ION DAMAGE IN ALUMINUM

ION - RUN	ENERGY MeV	RESISTIVITY $10^{-7} \Omega\text{cm}$	DAMAGE RATE $10^{-21} \Omega\text{cm/ion}$	DAMAGE RATIO PEAK / OPEN		DAMAGE RATE NORMALIZED TO ALUMINUM	DAMAGE ENERGY NORMALIZED TO ALUMINUM
				EXP.	THEORY		
Mg 4A	4.6	3.931	2.376	11.3	11.5	0.76	0.82
Al 1	4.8	3.914	3.059	10.2	11.1	1.00	1.00
Al 5	4.8	3.944	3.232	10.6	11.1	1.00	1.00
Si 2A	5.0	3.918	3.476	9.7	11.3	1.10	1.13
P 3A	5.3	3.921	4.201	9.5	10.8	1.34	1.31
S 3B	5.5	4.094	4.452	9.0	10.3	1.42	1.46
S 3C	5.9	4.256	3.503	9.3	10.9	1.11	1.37
Cl 2B	5.6	4.129	5.224	8.3	9.5	1.66	1.70
Ar 4B	6.0	4.188	5.392	8.1	8.9	1.71	1.97

TABLE V-II. MeV SELF ION DAMAGE RATES IN Al

Specimen No.	Thickness μm	Ion Energy MeV	Damage Rate $\Omega\text{cm/ion cm}^{-2}$ $\times 10^{21}$
10	.38	5.0	5.03
9	.25	5.0	6.95
15	.49	5.0	6.41
		4.8	6.26
		4.6	6.12
17	.44	4.6	6.79
25	.35	4.8	4.53

TABLE V-III. EXPERIMENTAL ION AND NEUTRON DAMAGE RATES IN Al
COMPARED WITH DAMAGE ENERGY CALCULATIONS

Specimen	Irradiation	Initial Damage Rates	Damage Rate Ratio ion/neutron	Damage Rate Ratio ion/neutron
Wire - 0.1 mm dia.	Fission Spectrum Neutrons	$2.13 \times 10^{-25} \text{ n/cm}^2 \cdot \text{n.cm}^{-2}$	2.35×10^4	2.50×10^4 (2.32×10^4) *
Thin Film 0.35 μm thick	Fission Spectrum Neutrons	$1.39 \times 10^{-20} \text{ n/n.cm}^{-2}$		
	4.8 MeV ^{27}Al	$3.27 \times 10^{-16} \text{ n/ion.cm}^2$		

* 20 eV threshold

NOGGLI Figure V-2

NOOTLE Figure V-4

NOBLE Figure V-6

NOG31E Figure V-7

NOGGLE Figure V-8

NOGGLE Figure V-9

SIMULATIONS OF HEAVY-ION IRRADIATION OF GOLD USING MARLOWE

R. Benedek

I want to tell you about simulations which we have been doing of the damage introduced into Au targets by heavy ions incident with energies in the range 20 to 50 keV. The work which I will be reporting was done in collaboration with M. O. Ruanlt at the Argonne National Laboratory.

We have used the Monte Carlo code MARLOWE to study the range and damage distributions introduced into Au by Ar, Fe, Kr, Mo, Xe, and Bi ions with three objectives in mind. First, we wished to compare the results obtained from the binary-collision simulations of MARLOWE with results obtained from transport theory, such as those reported by Brice, and by Winterbon. Next, we wished to compare the simulations for amorphous and crystalline materials, and last, we wished to study the relationship between the single cascade damage distributions, and the overall damage distribution.

Our MARLOWE runs were carried out with 100 to 200 incident projectiles (cascades) in each case, and the data was placed on a disk file. The data was subsequently analyzed further, as indicated in the flow diagram of Figure VI-1. The left hand leg of the flow chart indicates analysis by the code MARDAT to obtain the spatial distribution averages over the cascades which would be useful in comparisons with transport theory calculations. On the right hand leg we indicate the capability of producing perspective plots of individual cascades through analysis by the codes PLCARD and ORTEP.

The calculations were performed in two different modes. The BULK-AMORPHOUS (BA) mode considers an amorphous target medium and the projectile start inside the material. The SINGLE CRYSTAL (SC) mode utilizes a single crystal target, with the beam tilted by $(15^\circ, 15^\circ)$ with respect to the (001) surface. In both modes the low energy parameters used were displacement threshold, E_d , 35 eV; cut-off energy, E_c , 35 eV; and recombination radius, R_r , 0. In this respect I must say that our main interest was in the spatial configurations of the cascades rather than the absolute numbers of defects. In an even more restrictive sense, we concentrated primarily on vacancies.

Figure VI-2 shows a typical depth distribution of vacancies produced by 20 keV Kr incident on Au. Both BA and SC calculations were carried out with 100 cascades in each case. In the crystalline case you can see there is rather low level long range tail due to channeling. The peak positions for the two curves are relatively coincident. Channeling does not seem to have a significant effect on the total defect production, but it simply gives rise to the long range tail. Not all of the individual distributions obtained using 100 cascades were as smooth and well behaved as those shown in the figure, so that it would be desirable to use a larger number of cascades. That should be feasible with version 11 of MARLOWE.

In our comparisons of transport theory with the simulations from MARLOWE we reached essentially three conclusions. First, $\langle x_R \rangle$ the projected range obtained with MARLOWE (BA) is "consistent" with transport theory (Winterbon, Brice). That is, the differences observed are of the order of what one would expect from the different

potentials employed, Moliere in the MARLOWE calculations and Thomas-Fermi in the transport theory studies.

Our second conclusion concerned the ratio $\langle x_R \rangle / \langle x_D \rangle$, where $\langle x_D \rangle$ is the average damage depth. From MARLOWE (BA) we find that this ratio falls in the range 1.0 to 1.1. The transport theory calculations give for the ratio, however, values in the range 1.2 - 1.4. I should mention that in the energy range considered here there were essentially no differences between the results reported by Brice and those reported by Winterbon for this ratio. Since these are relative numbers there might be some significance in the differences between the two types of calculations.

With regard to straggling we calculated both range and damage straggling, and both longitudinal and transverse straggling. Our third conclusion is that the relative range and damage straggling obtained from MARLOWE, as expressed by the ratios

$$\frac{\langle \Delta x_R^2 \rangle^{1/2}}{\langle x_R \rangle} , \frac{\langle \Delta x_D^2 \rangle^{1/2}}{\langle x_D \rangle} , \frac{\langle x_{RT}^2 \rangle^{1/2}}{\langle \Delta x_R^2 \rangle^{1/2}} , \frac{\langle x_{DT}^2 \rangle^{1/2}}{\langle \Delta x_D^2 \rangle^{1/2}} ,$$

is in "reasonable" agreement (~15%) with the results from transport theory. We didn't discover any significant differences in these comparisons as a function of reduced energy.

In our comparisons between the amorphous and crystalline simulations, we found as expected that $\langle x_R \rangle$ is larger in the crystalline case. However, the excess in this parameter is considerably larger (~50 to 100%) than one might expect, since we intentionally chose a nonchanneled direction for the incident beam. A great deal of the channeling which does occur is not in the (001) direction.

but the considerably larger tail in the crystalline case is definitely due to channeling effects. The mean damage depth, on the other hand, is not very much affected by the channeling. The reason for this is that the "tail" in the crystalline case accounts for < 5% of the total defect production.

Table VI-I shows a comparison of the calculations of the peak location in the damage distribution by both transport theory and the MARLOWE simulations with experimental results obtained from stereo microscopy. Most of the results were obtained by Ruault, but the bismuth results are from recent work by Jager and Merkle of Argonne. Overall the agreement is reasonable.

ROBINSON

Roy, what are the units in that table?

BENEDEK

The units here are all in angstroms.

That gives you some idea of the uncertainties in trying to make a critical comparison of the calculations with experiment, since it is very difficult to measure such small projected ranges with sufficient resolution to make a sharp test of the theory.

We would now like to look into the differences in the damage distributions and in individual cascades. One measure of the differences in size is a parameter we call the radius of gyration, R_g . The parameter R_g is defined as

$$R_g^2 = \overline{Ax^2} + \overline{x_T^2} \quad . \quad \text{VI-1}$$

In other words, R_g is the root-mean-square displacement of a vacancy from the centroid of the damage distribution.

Table VI-II shows the resultant values of R_g for the total distribution, i.e., the sum of all the individual cascades, and for the individual cascades. The latter value for R_g is obtained by calculating R_g for each cascade and then averaging these values over the cascade histories. The difference between the distribution value and the cascade value of R_g is a measure of the spatial distribution of the cascades, i.e., of the manner in which cascades occupy the total damage region. The cascade contraction factor, δ , is given by

$$\delta = R_g^2(\text{cascade})/R_g^2(\text{distribution}) \quad \text{VI-2}$$

From the table one can see that the values of δ given by Sigmund, et al., are somewhat smaller than the values obtained from MARLOWE.

One of the ways in which this information can be useful is in determining the defect density. If one takes a cascade volume to be

$$V_C \approx 4\pi R_g^3/3 \quad \text{VI-3}$$

and the number of vacancies per cascade is N_V , then the defect concentration, C_V , is given by

$$C_V = 0.6 N_V/V_C = 0.143 N_V/R_g^3 \quad \text{VI-4}$$

In Eq. (VI-4) the extra factor 0.6 is usually employed to take into account the fact that all of the defects do not lie inside the volume V_C . Figure VI-3 shows values of C_V as calculated by MARLOWE plotted as a function of the energy density, as defined by

Sigmund, et al. This latter quantity is the energy per target atom per incident ion which is deposited in the core of the damage cascade. It is not clear precisely how these two quantities should be related, however, it can be seen that they tend to vary more or less together.

I would now like to direct your attention to some anomalous cascades which occur in the output from MARLOWE, and which indicate the wide variety of individual events which combine to produce the rather smooth damage distributions which are usually discussed. These cascades are shown in Figures VI-4 through VI-9.

Figure VI-4 shows results for a particular 10 keV Bi ion incident on Au. The circles are vacancies and the bar connections give you an indication of the nearest neighbor lattice sites. The crystal surface coincides with the x-y plane, and the parallel piped gives the smallest box which contains the entire cascade. The lengths of the box sides are indicated on the figure in lattice spacings, which for gold is about 4.08 Å. Thus, the sides of the box are all about 40 Å long. The primary ion entered the crystal at the point on the x-y plane indicated by the solid circle, and its momentum was approximately normal to the (001) direction. The defect density here, as measured by Eq. (VI-4), is about 8%. If you take the entire volume of the box shown in the figure and divide it into the number of defects you get a value of 4%. It is thus clear that there are a number of ways in which the defect density could be calculated, and the value of interest for a given application depends on the nature of the application. For example, somewhere in the central part of the cascade one could easily find

regions with a defect density of 50% or so. This cascade is probably a "normal" cascade.

ROBINSON

I would just like to comment here that because of the relatively high cutoff energy, 35 eV, you will not see the strong (110) linearization due to the replacement collision sequences. You will see a few of them, but this is a relatively high cutoff energy for that type of event.

BENEDEK

That's right. I have to say again, however, that this represents some rather preliminary work, and we really need to do a more detailed study of all the features of the cascades before making strong claims about the various features observed. We are hoping to also be able to show on plots such as these the interstitial distributions as well as the vacancy distributions, but that's for future work.

ROBINSON

What was the screening length in these calculations?

BENEDEK

The Firsov value.

Figure VI-5 shows a rather anomalous event for a 10 keV incident R_i ion. The long track seen there is almost (211), although these are vacancies, and not the projectile itself. The front face again is a (001) plane. The depth of this cascade is about four times the depth in the previous figure for the "normal" cascade.

NOGGLE

About what frequency do you observe these "pathological" events?

BENEDEK

About one in a hundred.

Now, it is often difficult to really be able to tell the true extent of a cascade from a single perspective plot. One way of getting around the problem is to make stereo pairs, and then to view them in such a way as to give a three dimensional aspect to the cascade. Another way of noting the various features of the cascade is to just take a substantially different perspective plot. Figures VI-6 and VI-7 show the results of the latter procedure for a 50 keV Fe cascade in Au. Figure VI-6 shows the cascade in the same perspective as the previous figures, and it is seen that no really unusual features are present in the cascade.

Figure VI-7 shows the same cascade as viewed from the upper face of the perspective in Fig. VI-6, i.e., looking down on the x-z plane. Now one sees that the cascade is in fact quite unusual. Apparently the projectile channeled, or almost channeled, from its entry point on the x-y plane to a point on the opposite face of the box, at which point it suffered a large angle scattering event. The recoil Au atom then created the damage region near the far face of the box while the scattered Fe atom created a damage track almost back to the y-z plane.

Figure VI-8 shows another unusual event for a 50 keV Ar incident on Au. It enters the crystal on the x-y plane, it causes a dense cluster near the far x-y face, and then it evidently channels across the box, creating another dense cluster near the y-z plane. The interesting point here is that the clusters are practically distinct.

The final figure, Fig. VI-9 shows a cascade for 50 keV Xe. The interesting point here is that the projectile makes a relatively dense cluster near the point of origin, then the track thins out and disappears, but there are then a few more defects formed near the end of the track.

ROBINSON

That looks like it was probably a planar channeled particle which was nearly channeled at the point where the track disappears. The particle then slowly crossed the plane, and then made some more defects near the end of track after which it was essentially dead as far as the calculation is concerned.

NOGGLE

What is the projected direction here?

BENEDEK

I haven't calculated it exactly, but it's close to a (112) direction again.

ROBINSON

It has been my experience that the axial channeling does not contribute significantly to events such as this. Usually when you see a long channeled trajectory, such as this, it usually is closely perpendicular to the $\langle 111 \rangle$ axis, i.e., in a (111) plane.

TABLE VI-1. COMPARISON OF PEAK DEPTH IN DAMAGE DISTRIBUTION IN PRESENT CALCULATIONS WITH OTHER THEORETICAL RESULTS AND EXPERIMENT

Ion	E (keV)	c	M_2/M_1	PEAK POSITION IN DAMAGE DISTRIBUTION					EXPT
				Brice	WSS (m=2)	WSS (m=3)	Marlowe		
							BA	SC	
Ar	50	0.19	4.9	92	100	60	100		95
Fe	50	0.12	3.5	73	70	55	60	60	80
Kr	20	0.03	2.3	28			35	35	40
Kr	50	0.07	2.3	60	65	50	40		65
Mo	50	0.06	2.1	55	35	50	70	40	50
Xe	50	0.04	1.5	47	35	45	40		45
Bi	10	0.004	0.94	12			25	20	40
Bi	20	0.008	0.94	19			30	30	40
Bi	40	0.012	0.94	31			35		

TABLE VI-II. RADIUS OF GYRATION AND CASCADE CONTRACTION FACTOR

Ion	E (keV)	ϵ	N_2/M_1	Radius of Gyration of Damage ($\text{\AA}$)					Cascade Contraction Factor ϕ		
				Winterbon	Marlowe				Sigmund et al	Marlowe	
					BA		SC			BA	SC
					Dist	Cascade	Dist	Cascade			
Ar	50	0.19	4.9	160			163	120	0.3		0.54
Fe	50	0.12	3.5	112	121	76	121	91		0.39	0.57
Kr	20	0.03	2.3	41	48	36	65	36		0.55	0.30
Kr	50	0.07	2.3	76			98	68			0.49
Mo	50	0.06	2.1	65	81	56	84	58		0.48	0.48
Xe	50	0.04	1.5	55			84	50	0.4		0.35
Bi	10	0.004	0.94		25	22	27	20	0.5	0.77	0.55
Bi	20	0.008	0.94	22	35	30	37	27		0.75	0.55
Bi	40	0.016	0.94	35			64	40			0.39

BENEDEK Figure VI-1

VACANCIES / INTERVAL

BENEDEK Figure VI-2

BENEDEK

Figure VI-3

BI105M4

BENEDEK Figure VI-4

BENEDEK Figure VI-5

BENEDEK Figure VI-6

FE502M5

BENEDEK Figure VI-7

BENEDEK Figure VI-8

MARLOWE CALCULATIONS OF RANGE DISTRIBUTION PARAMETERS: DEPENDENCE ON
INPUT DATA AND CALCULATIONAL MODEL

M. T. Robinson

I want to present some comparisons of range distribution calculations carried out with MARLOWE, with a goal of determining how the various input parameters and initial conditions affect the results. In this respect the work I will be talking about is somewhat similar to that just presented by Roy Benedek, although we have investigated a somewhat different set of comparisons, and also used a slightly different version of MARLOWE.

The specific example which I will discuss is 100 keV ^{196}Au incident on Au. This projectile is produced by $(n, 2n)$ reactions in Au, and 100 keV is about the average recoil energy obtained from the neutrons produced in the $^9\text{Be}(d, n)^{10}\text{B}$ reaction with 40 MeV deuterons. The calculations were done over the past couple of years in support of experimental studies by Jim Roberto of our laboratory. He is measuring ranges by the standard type of recoil-radioactive foil type of measurement. I will not present any comparisons with experiment, but I do wish to talk about comparisons of ranges calculated with a variety of MARLOWE parameters.

In the calculations, in every case, we have used the Moliere potential with a screening length of 0.0752 Å, which is a little larger than the Firsov value, and it represents a Robinson-Torrens quasistimate. The inelastic energy loss is normalized under conditions of the impulse approximation, i.e., at high energies, to the LSS k-value. In its latest versions MARLOWE has the

capability of using a local, i.e., impact parameter dependent, inelastic loss law as well as the nonlocal, or continuous slowing down law. Our calculations have used both the local and nonlocal versions of the inelastic loss as well as a combination of the two with the loss partitioned equally between them, i.e., an equipartition loss law. This does not mean equipartition in the Lindhard sense where the equipartition refers to the type of inelastic loss process rather than a mixture of two types of inelastic loss law. The particles always start in the calculations from a lattice site in an infinite medium, and with an isotropic distribution.

Table VII-I shows some of our results. The calculations are for monocrystalline targets, but with projectiles incident along "random" directions. The first column indicates the thermal condition of the target, and one should note that static and 0 K refer to distinctly different vibrational conditions for the target atoms. The second column indicates the type of inelastic energy loss law which was used, and the third column lists the number of histories calculated under the given conditions. The range distribution parameters which result from the calculations are tabulated in columns four through seven. The mean penetration is normalized by the lattice constant, the relative variance is the variance divided by the square of the mean, and the skewness is the third central moment divided by the variance to the three-halves power. The kurtosis, as I define it, is the fourth central moment divided by the square of the variance minus three. Thus, both the skewness and the kurtosis are zero for a gaussian distribution.

The first set of three entries in the table shows how the various range distribution parameters depend on the nature of the inelastic energy loss law. I remind you that at high energies the inelastic losses will be the same for all three models, since we have normalized it to be that way. At low energies, however, the impact parameter dependence of the inelastic losses is seen to have a significant effect on the resultant parameters. The increased range for the local model occurs because the deflection of the projectile by the elastic interaction excludes collisions with small impact parameters, and thus effectively reduces the inelastic stopping power. I will talk a little later about the large changes which are seen in the higher moments of the distribution, but I just wanted to point out at the outset that the results one obtains are dependent on the inelastic loss model, and it is not clear which one, if any, is the preferred model. Just to illustrate the origin of this effect, however, consider a channeled particle. In the local model there is essentially no inelastic loss, so that the particles just go on and on for quite large distances, eventually being stopped by the elastic losses. For the nonlocal model, however, all particles have the same inelastic loss, independent of their location in the channel, and thus they rapidly come to rest, all essentially at the same location. Both of these extremes seem quite unphysical, and thus the equipartition model would seem to be the best choice of the three.

The next set of four calculations shows how the various range distribution parameters depend on the lattice temperature. The first line is for a static lattice which is not the same as 0 K

which includes the zero-point vibrations. All the calculations for this set used the equipartition inelastic loss model. The static case here is also an independent statistical sampling, nonoverlapping with the static case in the first three lines of the table. The difference in mean penetration in the two equipartition-static cases results from the statistical scatter which occurs in this type of calculation and although the difference lies outside the sample error bars these results are typical. The Debye theta-value used here was the experimental value. We notice that the mean range increases with increasing temperature, while the relative variance increases, and then decreases as temperature goes up. You can immediately guess that the effect being observed here is that there is some blocking which tends to decrease the mean range. As the temperature goes up the blocking probability goes down, accounting for the trend observed in the results.

Now, the large skewness and kurtosis values, which I remarked on earlier, are due to channeling effects, as might be expected from the comparisons of the results for crystalline and amorphous targets. Figure VII-1 shows a comparison of the actual distributions in range obtained from the calculations for both cases and as a function of temperature for the crystalline case. The particles all start at zero, and the areas of the several distributions have been adjusted to give the same number of particles. The tails of the distributions have all been multiplied by a factor of eight for better viewing, and the 1% level is indicated on each distribution. This is the depth which is exceeded by 1% of the incident particles.

In conclusion then, I would say that people should be somewhat careful in using codes such as MARLOWE for such calculations because of the sensitivity to model parameters including, for example, the models of energy loss and models of thermal vibrations, etc. The fact that there seem to be some crystalline effects may also be important in that one should be careful in comparing amorphous and polycrystalline theoretical calculations with experimental results. Real materials are polycrystalline, and it is possible to do calculations with codes such as MARLOWE which purport to be applicable to polycrystalline materials. Whether some sample of target material really conforms to the model used in such calculations is, of course, anybody's guess.

Table VII-I. Range distribution parameters; dependence on calculational model. 100 keV $^{196}\text{Au} \rightarrow \text{Au}$.
Moliere potential, $a_{12} = 0.0752 \text{ \AA}$. Inelastic loss normalized to LSS theory.

			Mean penetrations m/a_0	Relative variance μ_2/m^2	Skewness	Kurtosis
Static	Local	1,000 atoms	25.54 $\pm$ 1.64	4.116	11.691	170.46
Static	Equipartition	1,000 atoms	23.04 $\pm$ 0.86	1.380	5.595	43.85
Static	Nonlocal	1,000 atoms	21.34 $\pm$ 0.67	0.8629	4.041	26.05
Static	Equipartition	2,000 atoms	21.58 $\pm$ 0.50	0.9078	5.602	49.65
0 K	Equipartition	5,000 atoms	22.82 $\pm$ 0.36	1.258	6.112	59.14
300 K	Equipartition	5,000 atoms	24.51 $\pm$ 0.35	1.028	5.190	46.70
1500 K	Equipartition	5,000 atoms	25.25 $\pm$ 0.25	0.5075	2.117	8.868

Winterbon's tables

using Ge $\rightarrow$ Ge, see the example of scaling on p. 47.

Density of Au = 19.29 g/cm³
 $a_0 = 4.07830 \text{ \AA}$

This gives:
 19.95 $\mu\text{gm/cm}^2$
 101.9 $\text{\AA}$
 24.98

0.2992 0.5477 0.162

100 keV $^{196}\text{Au} \rightarrow \text{Au}$

ROBINSON Figure VII-1

DISCUSSION SESSION

PRICE

Well, after all the results we have seen today, perhaps we should spend some time trying to see if we can reach some sort of consensus concerning just what the problems are, and whether or not we might recommend some future research, either theoretical or experimental, on these problems. Since Dick More is more or less in charge of collating our conclusions I think I will turn this session over to him.

MORE

What I would like to do first is to attach a number, that is an uncertainty, to the straggling parameter, ΔR_p . I don't want this number to reflect bad calculations, but I want to know if we can agree as to how accurately we can determine this parameter. In terms of the best calculations, which all have uncertainties, I would like to know how accurately we can know this quantity right now.

PRICE

Do you mean to include just the calculational uncertainties, or are the experimental uncertainties also included in the uncertainty?

MORE

No, I think the net uncertainty to which theory can predict this number, ignoring altogether experimental results.

ROBINSON

I think that there are two different problems which have to be addressed separately. The first is "how accurately does the theory

predict the mean penetration?". Now with regard to the Monte Carlo calculations this the mean penetration uncertainty has two components. One of these is a statistical one which is related to the number of histories one considers, and the other is related to the values of the parameters which one uses. One doesn't know what parameter to use. If you are satisfied, as seems to be the case in most calculations, that most theoretical methods give about the same mean penetration when the same potentials and stopping powers, etc., are used, then the only other problem is how accurately one can determine the relative magnitude of the straggling. That is the critical question. It doesn't matter so much what the actual magnitude is, but whether the theoretical procedures give a correct estimate of the amount of straggling which occurs for a given penetration depth. That is what really tells you the shape of the distribution. It doesn't matter if the mean is off a little bit, since this probably reflects the choice of input parameters.

As to comparisons with experiment, well that is also somewhat uncertain. I don't know of any really critical comparisons of the MARLOWE calculations with experiment. In my calculations as long as the target is amorphous, (and I didn't talk about it earlier) the relative straggling is more or less independent of the parameters which are input for the inelastic losses. In that case the relative variance changes by 3-4% or so, but when you start including the crystal effects then the relative straggling varies all over the place, and uncertainties in the input parameters become very important.

MORE

So actually, the great uncertainty is not what MARLOWE does with the information input to it, but what that information actually is.

ROBINSON

Sure, I think that's a correct statement. And, that applies to the other codes too. MARLOWE is an atomistic code, and in that sense it probably has a better physical basis than the continuum calculations; and within the transport theory spectrum there are a number of different codes using a variety of approximations with EDRP being sort of the end of the line, in the sense that it tries to do everything as simply and efficiently as possible. But MARLOWE also contains a number of approximations. It is a binary collision code, and one should probably be using an integral calculation for these problems, or at least for some parts of them. Also, thermal correlations, which are known to be important in some cases, are not included.

MORE

Well, what can we say that the uncertainty in R_p is, including the uncertainty in the input and the various approximations used in the codes?

BRICE

Well, on the average I would say about 40%, with maybe 20% uncertainty in the relative variance.

HAGGMARK

Well, it depends on the system being discussed; some systems are better known than others.

ROBINSON

It also depends on the energy range. At high energies you can probably do quite well.

MORE

Let's restrict it to the low energy range of interest in most current ion implantation type studies.

ROBINSON

Maybe then 20% is a safe estimate for the relative variance.

MORE

Anyone else want to vote on this?

MUELLER

I'll go 40%, I don't believe 20%.

MORE

I'm not sure that this is an acceptable procedure for a scientific conclusion. We won't be locked in on any number, I'm just trying to get some idea about what we feel in general. I'm trying to get something that's specific and simple that might be included in any statement which would come from this meeting. Well, what? Do we agree on 20 to 40%? OK, that's it. Now, what would we say is the largest uncertainty in the calculation of range and straggles? Is it in the collisions? Post collision energy transport? Where is it? Is it the potential?

MUELLER

I'd say that in terms of the range that the largest uncertainty is in the inelastic energy losses.

ROBINSON

Yes, I'd go along with that.

BRICE

And probably the distribution of charge states is the biggest uncertainty in the relative straggles.

CHOYKE

What's the best potential?

ROBINSON

I'm perfectly happy with the Moliere potential.

MORE

Let me throw out another idea. This is all my own words, but let's see what you think. I think there is a need for a flexible, user-oriented code designed for the smaller machines which can accept various elastic and inelastic loss laws so the user can play around with those two quantities.

ROBINSON

TRIM would meet that, if it could be available with adequate documentation. This is not yet true of the versions I have seen.

HAGGMARK

Biersack is writing that up now.

MORE

Another remark in this respect. Such a code does not want to use the first order version of transport theory, since we have agreed that that is the source of some of the problems with straggles calculations.

ROBINSON

TRIM is atomistic, so there is no problem there.

HAGGMARK

I didn't mention it earlier, but TRIM is a small code, about 200 cards I think.

ROBINSON

Yes, it's a tiny code. MARLOWE is about 6000 cards.

MORE

I'm a bit worried whether we have enough time to spend on the relative merits of the various codes. That might take a whole day, in order to be fair. We shouldn't recommend one code over another. Perhaps we should recommend that some funding agency support the writing of a code which meets the needs which we have so far discussed.

MUELLER

If you are looking for a code to replace EDEP-1, then TRIM is not it. It's too slow. What you want is something that runs as fast as EDEP-1, but is better. You can certainly do better.

BENEDEK

Let me say that for people who have mini-computers time really is not that important. I have run TRIM on the mini-computer in my office, and you can just start it going and let it run for days. TRIM runs about 30 times slower on an HP-2100 minicomputer than on an IBM-370.

MORE

Let me toss out another sentence which might appear in the write-up, and everyone will be given a chance to cross it out if they don't like it. "This group recognized that the theory of ion ranges has an important impact on planning experiments in many laboratories. It's important in semiconductor and fusion energy

technology." Now, here comes the dangerous part. "It is not receiving sufficient support because this work falls between institutional responsibilities." What ought to be done, I think, is that some funding agency ought to support the development of some new code which avoids many of the problems which we have discussed.

ROBINSON

Most of us here are DOE supported. Within the DOE area this problem does tend to fall in the cracks. That maybe leads to some problems. I would think that maybe BES should be supporting work of this character. Not fusion energy or solar energy, or you name it, some particular program. It is basically a problem that is of fundamental scientific interest.

MORE

If we are going to put out a statement that this meeting was held and we discussed certain problems it probably wouldn't be a good idea to just say that. Is there some way of saying that without saying that? We really shouldn't be telling any DOE organization what they should be doing, but perhaps we can suggest the same thing in more delicate language, to sort of summarize the conclusions we have reached here.

ROBINSON

It would be nice to have a sort of dial-a-code for the use of the experimentalists. Most codes, however, are such that they have to be used with some theorist looking over the user's shoulder... It's extremely difficult to use someone else's code. If you are going to use a code often it probably would pay you to write your own, even if you duplicate the efforts of some other person.

MORE

Well, if you are in a small lab where you, maybe, have one-fourth of a slot for a theorist then you really don't want to write your own code, but you need something available to aid in planning your experiments.

ROBINSON

Well, a 200 card TRIM code would seem to meet your requirements.

BENEDEK

TRIM is a very flexible code, and when it's published I don't see why any experimentalist couldn't use it. Especially when you use the path-length stretching feature.

HAGGMARK

That's an automatic feature. You have to bypass that if you want not to use it.

MORE

But can you do a calculation at 25 MeV and not require some large multiple of 25 minutes?

HAGGMARK

Sure. I've run 10000 particles of 3.5 MeV helium on iron, and it took about 1 hour.

MORE

But I hesitate to estimate the time that would take on a smaller computer.

HAGGMARK

But I wanted the details of the distribution. If I had just wanted R_p and ΔR_p I could have used 1000 particles to get a very accurate result. That's 5 minutes or so. A quick rough measure of the mean penetration can be determined with only 1000 particles.

MORE

Should we say in our statement that several codes exist which have the potential to be developed into a flexible user oriented code, but that support is needed for further development? Is that a true statement? For example, how long will it be before the TRIM code is widely available?

HAGGMARK

Biersack and I have agreed that he will be in charge of making the code available up until the time that the manuscript is published. It's almost ready to be submitted now. This is so that there will not be several versions of the code floating around.

MORE

Well, we don't seem to be reaching any definite conclusion concerning a consensus. If you have some afterthoughts about what you would like to see in a summary statement of this meeting, please send them to me or to Dave Brice. Nothing will go out before everyone has had a chance to look it over and approve it.