Machine Simulation of Collisions Between a Copper Atom and a Copper Lattice*

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We have examined a number of collision events in which the target atom is embedded in a crystal lattice. The fcc <100>, <110>, and <111> orientations were examined in detail for the energy range from 25 eV to 10 keV. Preliminary results for the bcc <100> lattice are included. Lattice effects are somewhat smaller than one might anticipate. Orientation effects are significant because the relative atomic separations vary considerably between different orientations. The general features of our results are insensitive to the form of interaction potential, but magnitudes vary considerably. For the Gibson No. 2 parameters in a Born-Mayer potential, lattice effects lose significance around 5-keV bombardment energy; for the Gibson No. 1 they persist to at least 10 keV. No "effective mass" behavior was detectable. Binary-collision theories are not valid for energies below a few hundred eV.

I. INTRODUCTION

RECENT experimental work[1–3] has begun to provide useful information on the ranges of heavy particles in metals. These results are valuable in the sense that they give information about the extent of the damaged area introduced by a single event, but they give little insight into the individual processes which combine to produce the event. There is a great temptation to describe these processes in terms of individual collisions, and to treat the history of a single event as a series of binary processes. This procedure is attractive because binary events are relatively easy to describe, but the binary collision assumption has never been properly justified.

Further information about crystal damage processes can be obtained from sputtering experiments,[4] and here also the trend has been toward the consideration of individual collision processes within the lattice. Henschke[5] has used this approach in his theory of sputtering and Harrison and Magnuson[6] have also applied it, with modifications, to a theoretical study of sputtering threshold energies.

The theoretical work performed by Henschke uses the momentum transfer concept initiated by Kingdon and Langmuir[7] to account for all the experimental phenomena observed at low incident-particle energy. To obtain this agreement he postulated an "effective" target mass in the two-body collisions. If the collision is between a surface atom and a moving ion or atom and is such that the surface atom is struck on its "interior" hemisphere, according to Henschke, an effective mass is not required and the two particles involved can be considered to have their actual masses. Should the collision of an atom or ion be directed inward from the target lattice surface, he proposes that the effect of the lattice can be simulated if the target atom is assigned a "very large" "effective" mass.

Robinson, Oen, and Holmes[8,9] have used digital computer techniques based on the assumption that the moving atom loses its energy through repeated binary elastic collisions, to make theoretical studies of the ranges, in solids, of atoms which have energies from 1 to 10 keV. The masses used in these calculations are the true masses of the interacting particles. The Brookhaven group has also taken advantage of the speed available with modern digital computers in the study of radiation damage.[10,11] They do not assume binary collisions but instead employ iteration techniques and Newton's equations of motion to solve the complex many-body problem. Although the computer programs are designed to study radiation damage, the basic principles involved are also important in sputtering.

If the binary collision model is assumed, cross sections or mean free paths, which describe the individual events, must be determined. As these parameters have never been determined experimentally, most calculations depend upon cross sections calculated from two-body interactions.[8,12] Excellent gas-phase experimental work on binary collisions is also available,[13] which could potentially be included in the theoretical models at some future time, if the binary collision approximation can be justified.

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† Lt. U. S. Navy, portions of this work were submitted in partial fulfillment of the requirements for the degree of Master of Science.

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[6] D. E. Harrison and G. D. Magnuson, Phys. Rev. **122**, 1421 (1961).

[7] K. H. Kingdon and I. Langmuir, Phys. Rev. **22**, 148 (1923).

[8] M. T. Robinson and O. S. Oen, Phys. Rev. **132**, 2385 (1963) and earlier papers.

[9] See D. K. Holmes, in *Radiation Damage in Solids* (International Atomic Energy Agency, Vienna, 1962), for a summary of the Oak Ridge National Laboratory theoretical work.

[10] J. B. Gibson, A. N. Goland, M. Milgram, and G. H. Vineyard, Phys. Rev. **120**, 1229 (1960), hearafter referred to as Gibson.

[11] C. Erginsoy, G. H. Vineyard, and A. Englert, Phys. Rev. **133**, A595 (1964).

[12] O. B. Firsov, Zh. Eksperim. i Teor. Fiz. **33**, 696 (1957) [English transl.: Soviet Phys.—JETP **6**, 534 (1958)].

[13] G. H. Morgan and E. Everhart, Phys. Rev. **128**, 667 (1962), and earlier papers.

Recent experiments by Veksler[14] indicate that lattice effects become important below 80 eV, but do not give any evidence which unambiguously requires on effective mass interpretation.

In this investigation we have undertaken a preliminary examination of the compatibility between the 2-body and n-body models in the energy range from 25 eV to 10 keV. We have chosen to examine one system in considerable detail, and have made comparisons, in so far as comparison is possible, between "free" binary collisions, and collisions in which the target atom is embedded in a lattice.

II. THE MODEL

A program was developed for the CDC-1604 computer which simulates a single collision event within a lattice. Our approach is similar to Gibson's model, but the microcrystallite is smaller, and we use a different method of calculation. We neglected all volume-dependent cohesive effects and all dissipative effects, and retained only the repulsive term of the potential function. These omissions can be justified in two ways:

(1) Our collisions are complete, in a sense to be discussed later, in relatively short periods of time (of the order of 5×10^{-14} sec in real time). In this time interactions with nearest-neighbor atoms of the target can begin, but these atoms acquire very little energy, or displacement, before we terminate the process. Effects produced in the collision have not propagated more than one lattice spacing away from the collision site before the collision is complete. Thus surface forces of the type used by Gibson do not have a chance to affect the interaction. Even if we should include cohesive forces they would remain a relatively small correction upon our results because of the relatively long times required for their action.

(2) All of our computations depend upon resultant forces which vanish unless an atom moves from its equilibrium position. Furthermore, all forces are suppressed until they exceed 10^{-11} N. [This force will produce an acceleration of approximately 0.1 (m/sec)/timestep.] With this approximation nearest neighbors enter the computations immediately, but next-nearest neighbors do not receive energies greater than 0.1 eV until approximately 40 timesteps. Except for the largest impact parameters, the complete collision normally takes about 20 timesteps. We examined various values of the force cutoff, and found that the collision dynamics were essentially identical for this and all smaller values. A larger cutoff may be possible, but we did not examine the possibility.

Our lattice is stable until disrupted by an additional particle. Once disrupted it will never restabilize because restoring forces have been omitted. We are not concerned about this instability because the events we study are complete before the instability becomes apparent, or alternatively, before the actual restoring forces in a real lattice would have time to act.

We considered four representative crystal samples, crystallites, three from the face-centered cubic system, and one from the body-centered cubic. The samples are cubes for the fcc (100) and bcc (100) runs, a rectangular parallelepiped for the fcc (110) section, and a more complicated section, for the fcc (111) sample. The fcc (100) and (111) samples initially contain 63 atoms, the fcc (110) and bcc (100) samples 35 atoms. To reduce the computation time we often remove the back plane, or even the back two planes, in cases where the front surface interactions are sufficiently complete before the deeper planes can be affected.

All of these atoms are capable of movement, if disturbed. The moveable atoms are surrounded on all sides by stationary immovable atoms positioned as a continuation of the lattice. In the course of a run the program maintained a continuous check of the energy transferred to these atoms; so that the crystallite size could be increased in a later run if the sample under study would not contain the event. The indicated samples satisfactorily contained all of the cases studied, and as noted above, could often be further reduced.

Four general categories of potential functions are currently under consideration by various authors.[8–12,15] The Bohr (exponentially screened Coulomb) function is

$$\phi_B=(Z_1Z_2e^2/r)\exp(-r/a_B),$$

with

$$a_B=a_H(Z_1^{2/3}+Z_2^{2/3})^{-1/2},$$

where the Z_i are the atomic numbers of the interacting atoms, e is the electronic charge, r is the internuclear separation, and a_H is the radius of the first Bohr orbit of hydrogen (0.529 Å). It is known to be too "soft" (the atoms can approach too closely) in the energy range below 1 keV. As this low-energy range is the region of primary interest in our work, we did not apply the Bohr potential.

The Thomas-Fermi-Firsov (TFF) potential[12] is

$$\phi_{\mathrm{TFF}}=(Z_1Z_2e^2/r)\chi(r/a_{\mathrm{TFF}}),$$

with

$$a_{\mathrm{TFF}}=1.123(Z_1^{1/2}+Z_2^{1/2})^{2/3}/a_H,$$

where $\chi(x)$ is the Thomas-Fermi screening function. Gibson[10] and Abrahamson[15] have examined the TFF function and found it too hard for separations greater than 1.5 Å and probably too soft in the range from 0.5 Å–1.5 Å. We have applied it for a few high-energy runs, but have not made detailed studies.

[14] V. I. Veksler, Zh. Eksperim. i Teor. Fiz. **42**, 325 (1962) [English transl.: Soviet Phys.—JETP **15**, 222 (1962)].

[15] A. A. Abrahamson, R. D. Hatcher, and G. H. Vineyard, Phys. Rev. **121**, 159 (1961); A. A. Abrahamson, *ibid.* **130**, 693 (1963), hereafter Abrahamson.

TABLE I. This table contains the numerical constants used for the major part of our computations.

Potential	A (eV)	ρ	E_{BM} (keV)	b_{BM}
1	0.0392	16.97	921.	−12.02
2	0.0510	13.00	22.5	− 9.211
3	0.1004	10.34	3.11	−10.34

Most of our effort was devoted to the Gibson forms[10] of the Born-Mayer (exponential) potential:

$$\phi_{BM}(r)=A\ \exp[-\rho(r-r_0)/r_0];$$

which can be put into the equivalent form,

$$\phi_{BM}(r)=E_{BM}\ \exp[-b_{BM}(r/l_0)],$$

where r_0 is the nearest-neighbor distance at absolute zero and zero external pressure (2.556 Å for Cu), and l_0 is half the cubic cell edge (1.804 Å for Cu). They consider three sets of parameters for ρ and A, see Table I. Potentials No. 1 and No. 2 are similar to those suggested by Huntington for Cu,[16] and No. 2 matches the Thomas-Fermi-Dirac (TFD) potential suggested by Abrahamson[15] near a separation of 0.5 Å (~2-keV energy), and crosses the Bohr potential near 0.3 Å (~6-keV energy). (See Fig. 2 of Ref. 10.)

If we accept Abrahamson's analysis,[15] the TFD potential is the most satisfactory approximation currently available. However, there is every indication that the TFD results are well bracketed by the Gibson potentials in the low-energy region which is our primary concern. For this reason, we have chosen to concentrate on the Gibson potentials and omit any consideration of the TFD.

All of our potentials consider only nearest-neighbor interactions. The Born-Mayer potentials vanish at the normal lattice internuclear separation, and the TFF potential can be "eroded" at this radius. To "erode" a potential, the value of the potential at the nearest-neighbor separation is subtracted from the value of the potential at smaller distances. The eroded form of the potential is assumed to be zero at separations greater than nearest neighbors.

Although our model of the microcrystallite would not contain the "voids" encountered by Robinson and Oen,[8] since our truncation radius is sufficiently large to completely fill the lattice, we feel that the eroded form is a closer approximation to the true situation in the lattice. It is important to note that "erosion" in our case differs considerably from the model used by Robinson and Oen.

The entire lattice is initially at absolute zero, since no vibrational energy is simulated. These approximations imply that the lattice has no potential or kinetic energy before interaction with the bullet, and all the energy in the lattice at any time thereafter is derived from the bombarding atom. Forces appear only when atoms move from their equilibrium position, or when another atom is introduced from the outside, which is the only situation considered in this paper.

The calculations do not follow a central difference method. Newton's equation of motion can be rearranged to give the change in velocity of a body acted upon by an average unbalanced force, $\bar{F}\Delta T/M=\Delta V$; and the change in velocity can be related to a change in position if an average velocity is assumed,

$$X_i(t+\Delta T)\cong X_i(t)+\Delta T[v_i(t)+\tfrac{1}{2}\Delta T\bar{F}/m].$$

The corresponding equation derived by the central difference method by Gibson *et al.* is

$$X_i(t+\Delta t)\cong X_i(t)+\Delta t[v_i(t-\tfrac{1}{2}\Delta t)+\Delta tF(t)/m],$$

where $F(t)$ is the resultant force acting on atom i at time t. If we make the replacement

$$v_i(t-\tfrac{1}{2}\Delta t)\cong v_i(t)-[F(t)/m]\tfrac{1}{2}\Delta t+\cdots$$

in this equation, it becomes

$$x_i(t+\Delta t)\cong X_i(t)+\Delta t[v_i(t)+\tfrac{1}{2}\Delta tF(t)/m].$$

Thus (to this order of accuracy), the only difference in the two methods will be in the treatment of $\bar{F}$ versus $F(t)$. In their paper Gibson *et al.* evaluates $F(t)$ at time t, while we calculate an approximate average value for F over the time interval.

Our average force is calculated by a double iteration procedure as follows: (1) assume an atom at position 1 with velocity 1; (2) calculate the total force on the atom as a result of all the other atoms in the lattice (this means normally only about 8–10 nearest atoms because the potential is eroded); (3) call this calculated force, force 1, and use the equation of motion to move the atom to a temporary position, position 2; (4) now repeat the force calculations for position 2, call this force 2; (5) go back to position 1, and use the average of force 1 and force 2 to move the atom to a new position, position 3. Procedures 1 through 5 constitute one "timestep." Forces are eroded in the same manner as potentials and are calculated by a subroutine based on the partial derivative with respect to distance of the potential function. Within the program all distances are measured in units of $\frac{1}{2}$ the lattice constant, which we refer to as the *lattice unit.*

The basic value of ΔT is dependent upon the original energy of the bombarding atom. ΔT is the time in seconds required for the incoming atom to traverse one lattice unit. The atom will lose energy as it interacts with the lattice, but ΔT remains unchanged. To add flexibility to the program, the basic value of ΔT can be multiplied by any desired factor (timestep multiplier). ΔT is established at the beginning of the program and is constant for the duration of the calculations.

We compared our average force method to the central difference method for several impact parameters and

[16] H. B. Huntington, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1958), Vol. 7, p. 213.

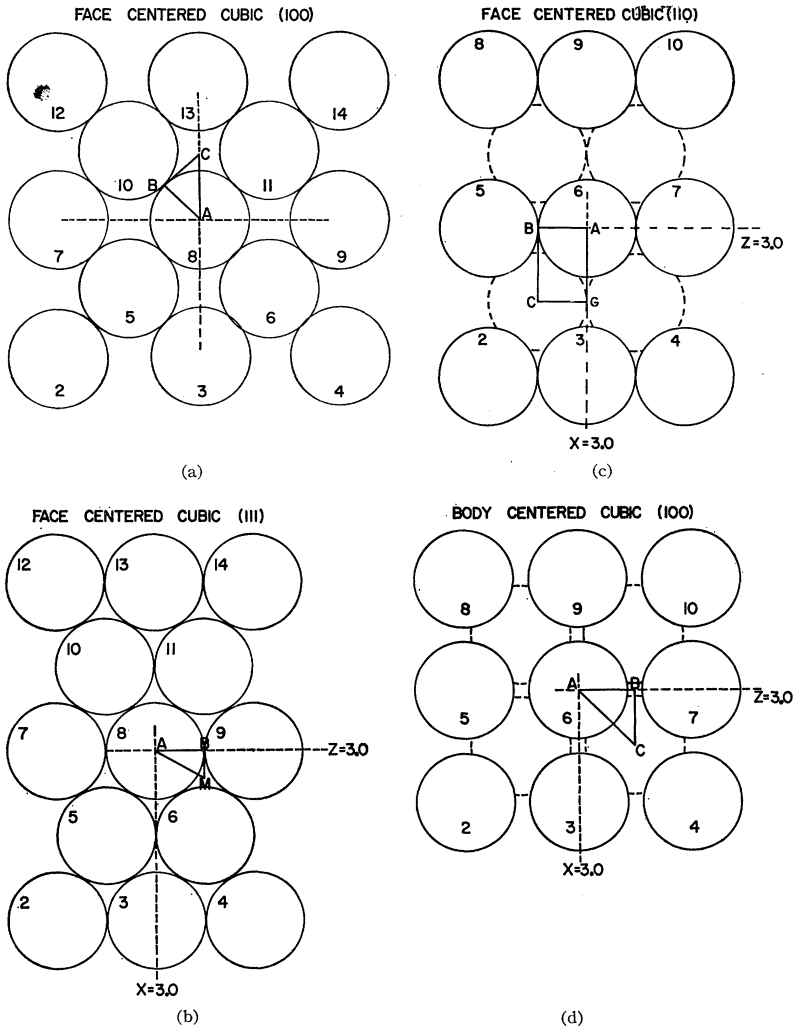

FIG. 1. The representative areas for each sample are indicated: (a) fcc (100), (b) fcc (111), (c) fcc (110), (d) bcc (100). These areas contain all possible impact parameter cases in all samples except the fcc (111). In our model there is a void in the second plane of the fcc (111) sample behind point M. We could also have considered the case where there is an atom in this location (a symmetric point across the line $Z=3.0$). We chose this case because the target recoil is more restricted for impacts near M than it would be for the symmetric point; so the lattice effects should be more noticeable.

various timestep multipliers. In all cases it gave a smaller percentage error in the final total energy of the system the central difference method run with one-half the corresponding timestep multiplier. The iteration process increases our computer running time, but the averaging process and the larger timestep multiplier cancel out the increase, and we are left with improved accuracy at no expense in time.

The bombarding copper atom is originally located in front of the $y=0$ plane and given a velocity in the $+y$ direction, which causes it to approach perpendicular to the face of the movable lattice core. The immovable atoms in the plane which covers the bombarded face do not interact with the bullet.

An impact area was chosen on a particular face so that points in this area would be representative of any point in that plane. An impact point is defined as the location on the face toward which the bombarding atom is directed. The bullet atom may or may not actually pass through this point. By moving in $\frac{1}{10}$ lattice unit increments, 36 impact points were assigned in the (100) impact "triangle." See Figs. 1(a) and 2(a). The (111) surface requires a right triangular representative area with the target atom located at the 30° angle, see Fig. 1(b). To reduce the computer running time, only 21 impact points were assigned, see Fig. 2(b). A rectangular impact area is more convenient for the (110) surface, see Fig. 1(c). The 36 impact points could not be so closely spaced, because the impact area is large compared to the other two cases, see Fig. 2(c). We also considered the (100) surface of an artificial bcc copper crystal in which the correct fcc interatomic spacing was retained. Again the representative area is a 45° isosceles right triangle.

The "central" lattice atom of the first plane, usually atom number eight, was assigned as the "target" in the many-body lattice problem so that its motion could be compared with the two-body problem. The geometrical relationship and physical constants of the two-body problem correspond to those of the incoming atom and "target" in the crystal.

The movement of atoms was continued until the

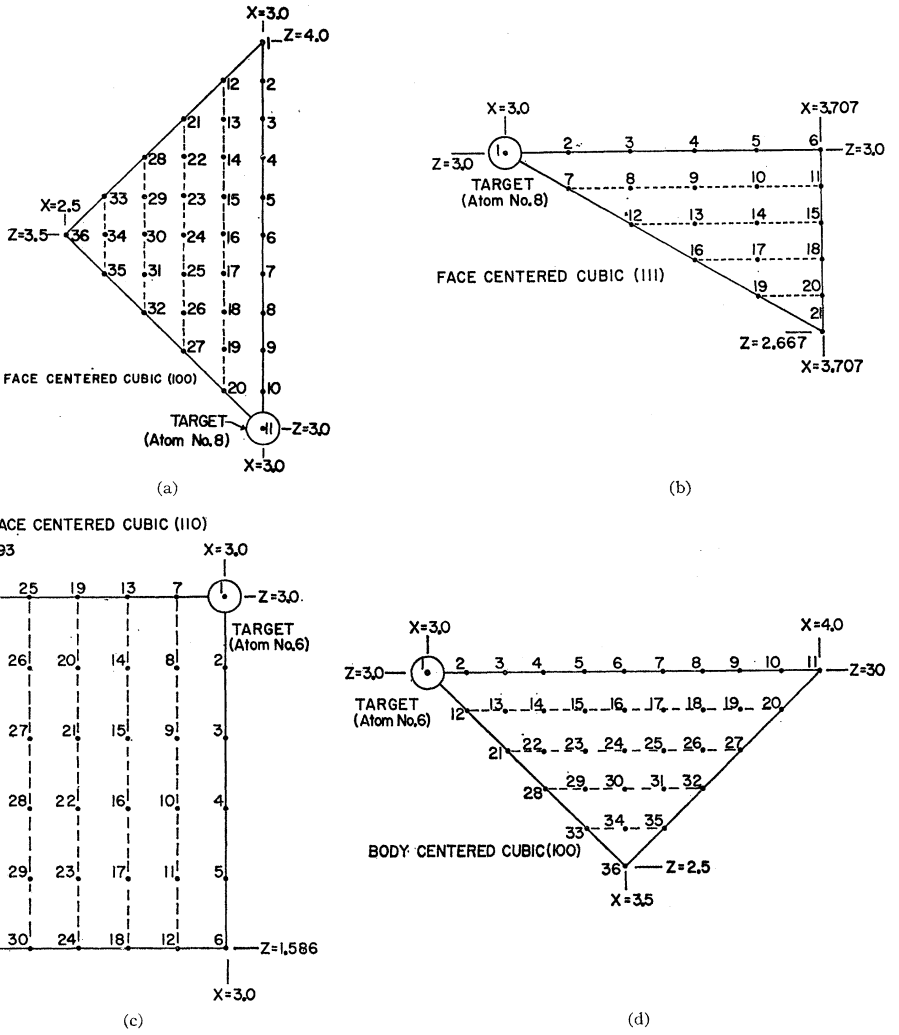

FIG. 2. The points probed by the program are indicated for each sample: (a) fcc (100), (b) fcc (111), (c) fcc (110), (d)fcc (100).

target atom reached a maximum in kinetic energy. At this point an energy balance was performed to determine the accuracy of the results. The percent error in total energy varied from about 5% at incoming particle energies below 25 eV to less than 0.03% at energies above 1000 eV. The error fluctuates about zero as the run progresses, and appears to be random rather than systematic. By the same process, the interaction was also performed with all of the lattice atoms suppressed except the target, to provide data on the comparable two-body interaction.

For each "run," the computer solves the many-body and two-body problem n times, corresponding to the n different impact points. The computer running time varied from 15 to about 30 min, and depended upon the values chosen for the timestep multiplier and the potential function constants. We originally assumed that the accuracy of the results would increase for smaller and smaller values of ΔT. We found that the value of ΔT which will give the minimum error in total energy appears to be a complicated function of the timestep multiplier, the incoming bullet energy, and the impact point. By trial and error methods, we found that below 100 eV for the Born-Mayer potential, a timestep multiplier of around 0.08 would produce reasonable errors at all impact points.

A. General Description of Event in the Lattice

The number of atoms disturbed in the lattice is a function of two variables: the number of timesteps the computer performs (elapsed time), and the impact point of the bullet. In general, the lattice is more disrupted by impact points in the area far from the target and is least affected by head-on collisions with the target. No more than half of the atoms are ever disturbed before the target reaches its maximum kinetic energy and usually only 5 or 6 acquire an energy greater than 0.1 eV.

The impact area is not symmetrically located with respect to the surrounding immovable atoms, but for equivalent points outside the impact area, excellent

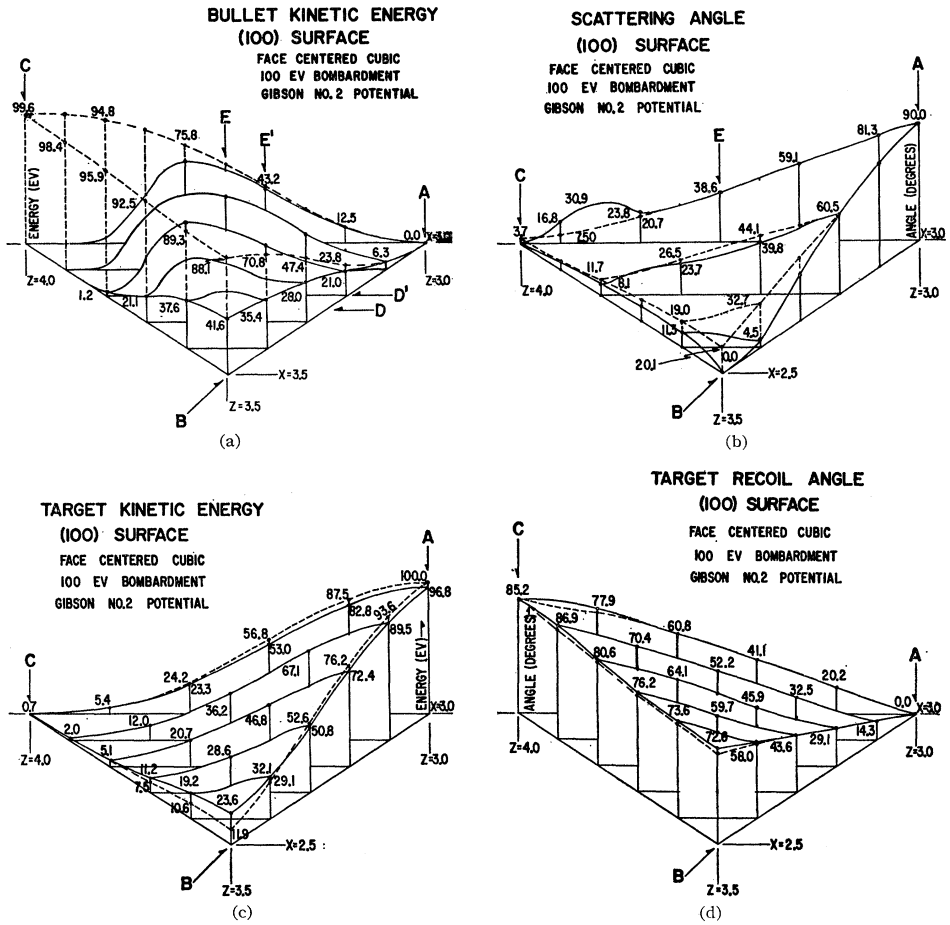

FIG. 3. Here we have a direct comparison of the lattice and two-body cases for various significant collision parameters in the fcc (100) surface. In this and succeeding drawings, solid lines refer to the lattice case, and the broken lines indicate the trend of the corresponding two-body data. Many of the binary collision points and the values at some lattice points have been omitted for clarity.

symmetry of displacement is observed for the movable atoms, which indicates that our microcrystallites are adequate for present purposes.

Because the collisions are complete in a relatively small number of timesteps, only a few atoms have significant kinetic energy when the interaction is stopped. These are normally the target, bullet, and the atoms directly behind the target and bullet in the lattice.

B. Comparison of Lattice Interactions with the Two-Body Interaction

A strict comparison of interactions in the lattice to the binary problem is not possible, but certain limited correlations can be made. The difficulty arises because the end of the interaction in the lattice cannot be defined explicitly. There are several criteria available that may be used in an attempt to compare the interactions. If the two-body interaction is allowed to continue until the potential between atoms is zero, for comparison purposes the lattice interaction could proceed until: (1) the potential between target and bullet is equal to zero, (2) the total energy (kinetic plus potential) of the target reaches a maximum, or (3) the kinetic energy of the target reaches a maximum. All of the criteria apply to the same physical situation in the two-body problem but are not equivalent in the lattice interaction.

We chose the maximum kinetic energy of the target as the comparison stopping point because this represents a time when the target and bullet have almost ceased to interact and are just beginning to interact with other lattice atoms.

The geometrical relationships of the target, bullet, and the lattice introduce complications into the comparison scheme. The motion of the target in the lattice is not restricted isotropically; so azimuthal orientation (around the surface normal) is a significant parameter. Restriction of the target motion lengthens the interaction time between bullet and target, and more energy is transferred to the target than in the two-body event. This effect is noticeable only at impact parameters of 0.5 lattice unit or greater. At smaller impact distances the interaction occurs so rapidly that the target motion is very small, and this lattice effect is reduced. The kinetic energy transferred at distances smaller than 0.5 lattice unit is less than that transferred in the two-

body case, because some target kinetic energy is immediately absorbed by the remainder of the lattice. The atoms behind the target in the lattice also play an important role but their effect is not so immediately obvious as those just discussed.

For a static system of two equal mass atoms with a conservative repulsive force between them, the total potential energy of the system can be halved and the result assigned as *the* energy of each atom; and, if the two atoms are allowed to move, the total energy (potential plus kinetic) of each will remain constant and equal to one-half the original potential energy. For any system such as our lattice, where the atoms are not static, this process which assigns energy to any one atom is not longer generally possible. As a matter of convenience for "bookkeeping" purposes the potential energy of an atom in the lattice is defined in the program as half the potential associated with its position. Of course, the target could eventually receive none of the potential energy or twice the indicated value. If we accept the indicated assignment of the potential energy, for head-on collisions the total energy of the target is approximately equal to the energy transferred in the two-body problem (within 2%) for energies greater than 50 eV. We have very clear evidence that this sharing procedure is generally much poorer than our results would indicate. Satisfactory results can be obtained by this method only when the bullet-target potential energy is small.

We specifically chose to define the completion of an event at the maximum of the target kinetic energy because this time gives the most favorable ratio of target kinetic to target potential energy. The uncertainty of assignment of potential energy cannot be removed, but its effect is minimized when the target kinetic energy is maximum. At completion the total bullet-target interaction potential energy rarely exceeds 5% of the original energy. This potential energy uncertainty dominates the entire computation and effectively sets a lower bound to the final uncertainty which cannot be significantly modified by increased computational precision.

It is possible to obtain much more accurate energy checks at low bombardment energies, but the increased accuracy is not justified because the potential energy uncertainty cannot be removed completely by any technique which is not expensive in computer time. When we also consider the uncertainties connected with the potential function a fast system with errors of the order of 5% seems more desirable than a slow system of greater precision but large uncertainty.

III. RESULTS

In this section we shall consider the Gibson No. 2 (Bory-Mayer) potential results in detail, and then indicate the differences which occur when the other potentials are used in the same geometrical situation.

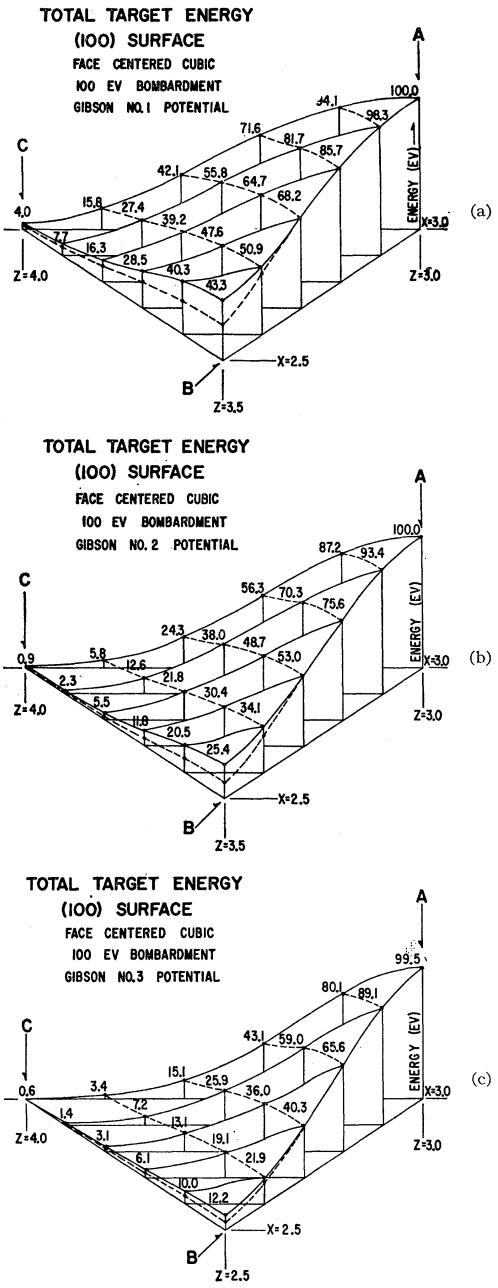

FIG. 4. In this figure we can see how the "total" target energy changes as the potential function parameters are varied. The potential function has little influence on shapes, but it does change numerical values. The solid lines are drawn from the lattice calculations, while the broken lines come from the binary collision case.

A. The (100) Surface

1. The Bullet

For bullet energies above 50 eV, in an impact area $AD'E'$ near the target atom, which comprizes only $\frac{3}{16}$ of the total lattice area, the n-body bullet's kinetic energy after the interaction, is within $\sim 10\%$ of the

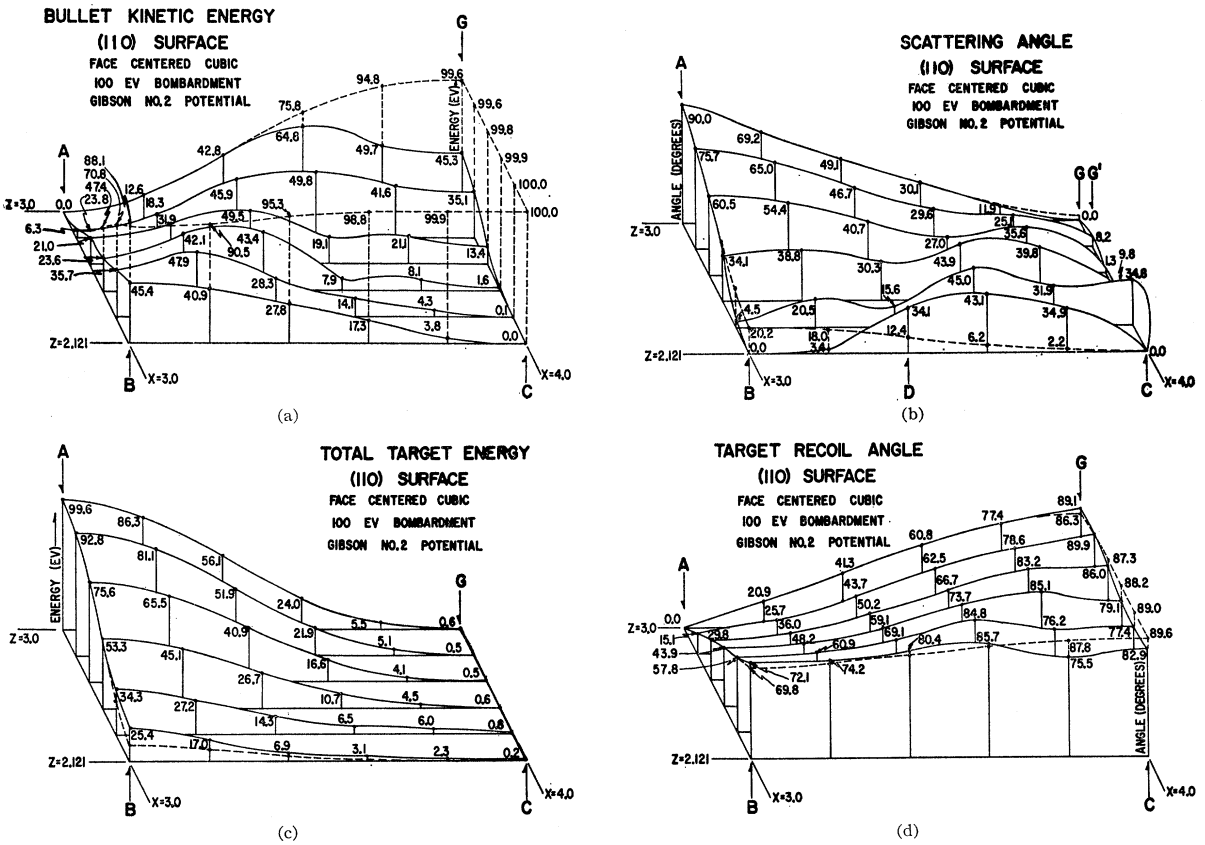

FIG. 5. This figure corresponds to Fig. 3, but refers to the fcc (110) section. As before the broken lines are the two-body results, and the solid lines refer to the lattice.

two-body result, see Fig. 3(a). Over the entire area the bullet's final energy is less in the n-body than in the two-body case, but only in the area $AD'E'$ can this loss be ascribed to lattice effects on atom No. 8, because in the rest of the impact area the bullet is engaged in relatively violent collisions with other members of the lattice. The region around B, the "double collision" point, is particularly instructive, because here the bullet is colliding simultaneously with two essentially equivalent targets. We see that the bullet's energy loss is more than doubled at 100 eV, and the effect is even stronger at lower bombardment energies. Thus in the region ABE, which is most characteristic of the interaction with atom No. 8, the bullet consistently loses more energy per interaction in the lattice than in a two-body event. Note that point C is a "quadruple collision" point.

The lattice has little effect on the scattering angle in the region ABE except for a small area near the double collision point B, where it is significantly reduced, see Fig. 3(b). The scattering angle is increased in the region BCE, and the relative increase increases with the bombardment energy. The line BC contains a maximum of the scattering angle which increases and moves toward C as the bombardment energy increases. Near C with a 1-keV bullet, atom deflections as large as 50° occur, but most of the bullet's energy is lost to an atom of the second layer; so these large deflections probably are not too significant. To the extent that "average" has any meaning under these conditions, the lattice appears to have little "average" effect for violent collisions.

2. *The Target*

Except for a small region near the double collision point B and along the line BC, see Fig. 3(c), the lattice has little effect upon the maximum kinetic energy transferred to the target in the bombardment energy range from 50 eV to 10 keV. In the excluded region, which comprises less than $\frac{1}{8}$ of the total area, the energy transfer is augmented. Near the double collision point is is approximately doubled for bombardment energies below 500 eV. At 100 eV this augmentation process produces a 25-eV transfer at B compared to $\sim$12 eV in the two-body case (Gibson No. 2 potential). For energies above 1 keV the augmentation is not longer significant and the energies transferred are less than 10 eV over the entire augmentation region.

As the energy is not clearly defined in the lattice, we also examined the total lattice atom energy, see Fig.

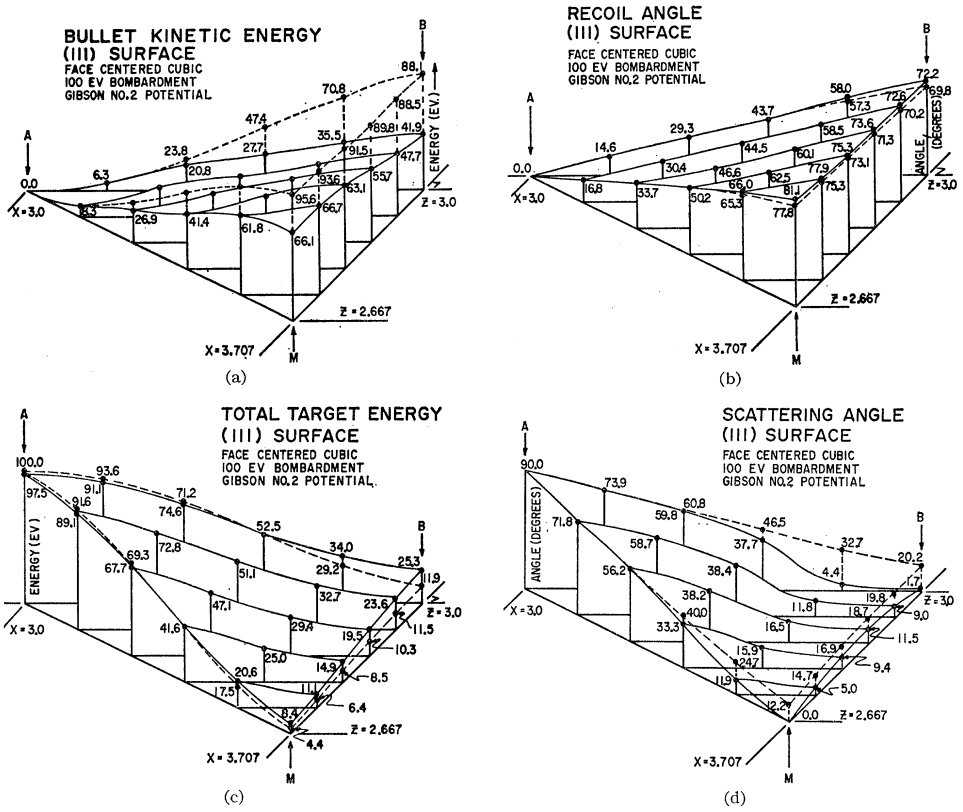

FIG. 6. This figure is similar to Figs. 3 and 5, but refers to the fcc (111) surface. As before the solid lines describe lattice calculation data, and the broken lines connect two-body points. Some numerical values are omitted for clarity.

4(b). Except for the *BC* region mentioned above, the target kinetic energy and the target total energy do not differ by more than 3% over the energy range from 50 eV to 10 keV. In the *BC* region the difference never exceeds 10%. *We conclude that the lattice has little effect upon the energy transferred to the target.*

At very low energies, below 100 eV, the lattice case recoil angle is augmented as much as 10% near point *C*, otherwise the lattice and two-body cases agree very closely over the entire area, see Fig. 3(d). The effect near *C* decreases at higher energies, and the recoil angle is reduced below the two-body value at energies above a few hundred eV.

3. *Potential Variations*

We shall refer to the Gibson No. 1 potential as the *hard potential*, because it produces a "large" atom and a high displacement threshold. The Gibson No. 3 potential will be our soft potential. It leads to "small" atoms, and a low displacement threshold.

The hard potential augments the energy transfer process for given impact parameter, and the soft potential reduces the transfer.

Figure 4 shows a detailed comparison of the "total" energy transferred at points in the (100) triangle for the different potential functions. As we would expect, the variation with potential parameters is large, but the special features of various points, as described for the No. 2 potential do not change significantly as the potential function is varied.

B. The (110) Surface

As far as possible the letters in Fig. 5 correspond to the equivalent points of Fig. 3. We note that the close-packed [110] chain which lies in the (110) surface tends to inhibit the energy transfer from bullet to target for points in the line *AB*, the [110] direction see Fig. 5(a). Slight displacements from this line give enhanced transfer compared to corresponding line in the (100) surface, because the perpendicular [110] close-packed chain of the (100) surface does not occur in the (110) case. The scattering angle is not significantly affected along the close-packed direction *AB*, but the region in which the lattice increases the scattering angle, *DCG'*, see Fig. 5(b), is larger than the corresponding area in the (100) case. As before, the lattice has little effect upon the total energy transferred to the target except in a region near the line *BC*, see Fig. 5(c). Here the relative increase is somewhat less than in the (100) case. We note that in ~60% of the (110) representative area the total energy transferred to the target by a 100-eV bullet is less than 20% of the bullet energy. This fraction is about 32% of the representative area in the (100) case. Thus on the average (100) targets receive more energy per surface collision, which may explain why the (100) sputtering ratio is larger than the (110) ratio.

C. The (111) Surface

As before, points A and B are equivalent to the corresponding points on the (110) surface, but here point M is a "triple collision" point, three simultaneous targets, which has no equivalent on the other surfaces, see Fig. 6. The behavior at the double collision point B differs from the corresponding points in the (100) and (110) surfaces, because the bullet is actually experiencing a modified triple collision through its interaction with atom No. 6. This effect is not so apparent in the energy figures, but it shows up very strikingly in the differences between Figs. 3(b) and 6(b). The scattering angle at B in the (111) surface is surprisingly large, and is in the positive Z direction. The target recoil angle is not significantly affected. The area around point M also requires comment. The entire region MB is a region of enhanced transfer, and the total energy transferred is much larger at MB points than at corresponding BC points in the (100) case. At 100-eV bombardment the region of energy transfer less than 20% is only 14% of the total area for this (111) case, while it was 32% of the (100) area. Scattering angles near M are smaller than those near C; as are recoil angles. The net effect of bombardment upon the (111) surface will be to produce more energetic particles which recoil at *slightly larger angles to the surface*. Thus, there is a higher probability that the second generation collisions, between atom No. 8 and some other lattice atom, will send the second atom "outward" from the (111) surface. This effect combined with the larger energy transfer probability should be sufficient to explain the increased sputtering ratio from (111) surfaces when compared to the (100) surface.

D. The (100) Surface of the bcc Lattice

1. The Bullet

As in the fcc case, the bullet kinetic energy is little affected in the region ADE, see Fig. 3(a). The double collision effect at point B is less pronounced because the two targets are more widely separated. Again, the kinetic energies in the region CEF are not significant, because the major collision is now with the atom below C in the next layer of the target. The scattering angle behavior is equivalent to the fcc (100) behavior, if we make allowance for the larger impact parameters required in the bcc case.

2. The Target

The lattice has no important effect upon the energy transferred to the target at any point in the entire impact area. The recoil angles are somewhat reduced in the region near C, but the effect is not significant because the energy transfer is so small in this region. The target behavior would be well characterized by the two-body behavior over the entire impact area at 100 eV.

3. Potential Variations

As we would expect, the hard potential makes the energetic and angular behavior of both bullet and target approach the fcc (100) surface behavior. Except at the double collision point, the soft potential case of the fcc (100) surface looks very much like the hard potential case of the bcc (100) surface. The energy transfer at the double collision point is markedly reduced in the bcc case because the targets are more widely separated.

The soft potential converts the bcc target into an essentially free body. Effects upon the target motion are completely neglegible.

IV. DISCUSSION

A. Effective Mass

For a head-on collision in the lattice there is very little geometrical effect, and an "effective" mass could be described. For computations made with the Gibson No. 2 potential at 25 eV, with copper bombarding copper, the mass of the target is apparently less than 1.6 times the bullet mass, and approximately $95\pm3\%$ of the energy is still transferred to the target. For a 100-eV bullet, the effective mass increase is not detectable. We used the program, as modified to observe chains and channels, and could find *no evidence of bullet recoil* which could be attributed to an "effectively heavy target" as proposed by Henschke.[5] Although an effective mass concept for the head-on collision is possible, it does not properly describe the subsequent motion of either target or bullet. If the bullet motion results in a glancing hit upon the target, no single effective mass can be assigned to the target because the behavior is a function of the impact parameter, *and its orientation*. An average effective mass is not applicable because the geometrical effects of the lattice on the direction and energy of the recoil atom are far more significant than the mass of the target.

These results apply to a collision anywhere in the lattice and are not limited to the interaction of surface atoms with incoming particles. The results indicate that Henschke's[5] "effective mass" concept and the rebound phenomena associated with it are not a good description of collision events in a lattice.

B. Low-Energy Sputtering

In certain respects our results can be compared with Veksler's[14] experimental work with molybdenum (bcc) targets. Our very low-energy studies were made with the fcc programs, and our bcc studies are based upon an hypothetical bcc copper crystal, but we have sufficient confidence in the goemetrical properties to venture a few comments on Veksler's interpretation of his data.

We cannot support Veksler's position with respect to the effective mass, but in all other respects his general conclusions are consistent with our work. This analysis gives good evidence to support his opinion that the

two-body collision model, based upon elastic hard core interactions, is not acceptable at low bombardment energies. More complete comparisons between theory and his experiments will not be possible until heteronuclear interatomic potentials for molybdenum are developed.

C. The Thomas-Fermi-Firsov Potential

Early in our program we attempted several high-energy runs (to 30 keV) with the TFF potential. As a result of Abrahamson's later work,[15] we did not pursue this line of research beyond the preliminary states. For 10-keV bombardment the TFF results are essentially equivalent to a Born-Mayer potential which is slightly softer than the Gibson No. 2, but not so soft as the Gibson No. 3. No effects are detectable, which can be attributed exclusively to the TFF potential function.

D. The Gibson Potentials

At this time it would be premature to suggest that a particular potential function should be adopted to the exclusion of all others, but of the few functions we have examined only the Gibson No. 2 leads to consistently reasonable results over the entire energy range from 25 eV to 10 keV. This is impressive behavior for a simple function which purports to describe such a complex interaction. Our calculations indicate that it is the best approximation available at the present time.

V. CONCLUSIONS

A detailed analysis of our results has not produced any particularly startling conclusions. Most of the qualitative features would be anticipated by anyone who undertook a careful study of a crystal model. Still, beyond some point, the qualitative behavior is not sufficient, and a beginning must be made with numbers. Because the numbers we have discussed come from a computer rather than an experiment does not mean that they are therefore correct. We have performed a set of experiments in a computer, based upon the best input data available, and subject to a reasonable set of compromises in the physical model. *The output should be treated as experimental results.*

Subject to these limitations, we found that the lattice has little effect upon the total energy transferred. Apparently the effective mass approach has no meaning, and we cannot replace the complex crystallographic interactions with averages.

We are forced to conclude that binary collision approximations will slightly under-predict the true energy transfers at all times, and will have the largest error for large impact parameter collisions where the total transfers are small, and therefore most sensitive to small changes. From our analysis we must conclude that the binary collision model will tend to reduce the number of displacements produced by a heavy ion, or under-predict the sputtering ratio for an external event. Differences between the binary collision model and the n-body model will be particularly apparent in the calculation of particle range distributions where large relative changes in small scattering angles and energy transfers are particularly significant.

Finally, we would like to comment upon the possibility of analytic theoretical studies of low-energy events. Our investigation clearly indicates that *all* theoretical research below approximately 500 eV must consider a more complex model than the binary collision approximation. Thus all analytic theories of the sputtering threshold, for example, [including one of the authors' (DEH) own[6]] are now suspect, and will require re-examination.