its value is

$$
\begin{aligned}
[\mathcal{H}_{\rm hfs}', M_z] = (g\beta_0/2) \sum_j
&\times\{(A_{xj}/A_{yj})[T_1^{(1)}(A_j\mathbf{S}_j)+T_{-1}^{(1)}(A_j\mathbf{S}_j)] \\
&\times[T_{-1}^{(1)}(\mathbf{I}_j)-T_1^{(1)}(\mathbf{I}_j)]+(A_{yj}/A_{xj}) \\
&\times[T_1^{(1)}(A_j\mathbf{S}_j)-T_{-1}^{(1)}(A_j\mathbf{S}_j)] \\
&\times[T_{-1}^{(1)}(\mathbf{I}_j)+T_1^{(1)}(\mathbf{I}_j)]\}.
\end{aligned}
$$

We now square the commutator and determine the trace of the resultant. The computation is much simplified by the fact that the only nonzero contributions to the trace arise from terms of the form

$$\mathrm{Tr}[T_M^{(1)}(A_j\mathbf{S}_j)^\dagger T_{M'}^{(1)}(A_k\mathbf{S}_k)]$$

and

$$\mathrm{Tr}[T_M^{(1)}(\mathbf{I}_j)^\dagger T_{M'}^{(1)}(\mathbf{I}_k)],$$

with both $j=k$ and $M=M'$. Thus

$$
\begin{aligned}
\mathrm{Tr}\{[\mathcal{H}_{\rm hfs}', M_z]^2\}
&= -(g\beta_0)^2 \sum_j \mathrm{Tr}[T_1^{(1)}(A_j\mathbf{S}_j)^\dagger T_1^{(1)}(A_j\mathbf{S}_j)] \\
&\quad \times \mathrm{Tr}[T_1^{(1)}(\mathbf{I}_j)^\dagger T_1^{(1)}(\mathbf{I}_j)][(A_{xj}/A_{yj})^2+(A_{yj}/A_{xj})^2].
\end{aligned}
$$

If the paramagnetic ions are assumed to be identical, i.e., $A_{xk}=A_x$, $A_{yk}=A_y$, $A_{zk}=A_z$, the result can be expressed as

$$
\begin{aligned}
\mathrm{Tr}\{[\mathcal{H}_{\rm hfs}', M_z]^2\}
&= -(g\beta_0)^2\, \mathrm{Tr}[\mathcal{H}_{\rm hfs}'(M=1)^\dagger \mathcal{H}_{\rm hfs}'(M=1)] \\
&\quad \times[(A_x/A_y)^2+(A_y/A_x)^2].
\end{aligned}
$$

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Partition of the Average Energy Deposited in Germanium as a Function of Incident Neutron Energy*

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The average energy deposited in crystalline germanium per incident neutron has been calculated as a function of neutron energy. The calculations are for neutron energies below 4 MeV, where scattering events predominate and charged-particle production is minimal. A calculation at 14 MeV by Nichols is also included. As the incident neutron energy increases from 50 keV to 14 MeV, the average ionization energy deposited increases from $\sim 1\times10^{-12}$ to $\approx 1\times10^{-8}$ (erg/g) per (neutron/cm^2), and the energy available for displacements (nonionization) increases from $\approx 1\times10^{-10}$ to $\approx 3\times10^{-9}$ (erg/g) per (neutron/cm^2). The calculated neutron energy dependence of the energy available for displacements agrees with the energy dependence of carrier-removal experiments in germanium performed with monoenergetic neutrons. Comparisons of these calculations are made with analogous ones for silicon. The energy deposited into atomic processes per carrier removed for ~ 40-Ω cm n-type germanium is $\approx 0.5\times10^{-9}$ erg/carrier, and the corresponding number is about a factor of 2 larger in the case of n-type silicon.

INTRODUCTION

A VERY significant amount of energy can be imparted to a crystalline solid through neutron reactions. A full understanding of neutron-induced effects requires a knowledge of the partition of energy between electronic and atomic processes. The energy going into atomic processes is available for neutron displacement damage, whereas the energy going into electronic processes is available for the production of transient ionization effects.

This paper is the fourth in a study of the partition of energy of energetic particles in crystalline solids. The first paper[1] (I) gave the ionization produced by an energetic silicon atom in a Si lattice. The second paper[2] (II) was a similar study for Ge. The third paper[3] (III) gave the partition of the average energy per incident neutron imparted to a Si lattice as a function of neutron energy. This paper is a study for Ge, analogous to III, and gives the partition of the average energy per incident neutron imparted to a Ge lattice as a function of neutron energy. A partial account of this work was presented in Ref. 4.

The model for the calculations was first presented in III and is reviewed briefly. This is followed by a presentation of the calculations. The calculations are then compared with carrier-removal measurements made in Ge as a function of neutron energy. The

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[1] A. R. Sattler, Phys. Rev. **138**, A1815 (1965).

[2] A. R. Sattler, F. L. Vook, and J. M. Palms, Phys. Rev. **143**, 538 (1966).

[3] A. R. Sattler and F. L. Vook, Phys. Rev. **155**, 211 (1967).

[4] A. R. Sattler, in *Radiation Effects in Semiconductors*, edited by F. L. Vook (Plenum Press, Inc., New York, 1968), p. 243.

paper concludes with a comparison of the present results with those for Si.

MODELS FOR CALCULATIONS

Neutron-induced events in a solid can produce heavy recoil particles, light-charged particles, and photons. It is these reaction products that transfer energy to the crystal. As in III, we neglect the ionizing effect of neutron-induced photons, considering, in effect, device-size Ge samples. (See the Appendix for a more complete discussion of the approximations.)

In order to calculate the energy partition as a function of neutron energy, a knowledge of cross-section data and the energy partition of the neutron-induced reaction products is necessary. There are enough total and differential cross-section data for Ge to make reasonable calculations over the fission spectrum. The energy partition of light-charged particles is trivial because virtually all of the energy goes into the electronic system. The energy partition for heavy Ge recoil atoms has been reported[3,5] and is based on measurements of the ratio of the number of pairs produced by a heavy recoil atom to those produced by an electron of the same energy. Such ionization data are interpreted to yield the partition of energy between electronic and atomic processes by assuming that the number of pairs produced per unit amount of energy going into electronic processes is constant and independent of the particle or its energy. Since an energetic electron loses virtually all of its energy to electronic processes, the measured ratios give, on the basis of this assumption, the fraction of the energy of the recoil atom going into electronic processes. Theoretical and experimental arguments in I, II, and III indicate that this assumption is valid, and it is this assumption that is the basis for predicting the partition of energy in the present paper. The term "ionization" therefore will be used in the rest of the paper to represent the amount of energy going into electronic processes.

Calculations were made over ranges of incident neutron energies E_n; 50 keV$\leq E_n \leq$1.5 MeV, and at 3.5 MeV. The production of heavy recoil atoms dominates in this energy region. Another calculation[6] of the energy partition has been made at 14 MeV, where charged-particle production is important.

The energy spectrum of Ge recoil atoms from neutron elastic and inelastic scattering is deduced from differential cross-section data at each neutron energy. The average energy partition results from II and Ref. 5 are folded into this energy spectrum. This gives the contributions of the Ge recoil atoms to the average energy going into ionization and the average energy going into atomic processes and hence available for the production of damage.

The average ionization per gram per incident neutron per cm^2 $\bar{I}(E_n)$, produced by recoils from neutron elastic and inelastic scattering in the region where these reaction cross sections virtually make up the total cross section, is

$$\bar{I}(E_n)=\frac{N}{A}\sigma_{\text{total}}(E_n)\langle Tf(T)\rangle_{\text{av}}$$

$$=\frac{N}{A}\int_{T_{\min}}^{T_{\max}}\sigma(E_n,T)Tf(T)dT, \quad (1)$$

where $T=T(E_n,Q,\cos\theta)$ is the energy imparted to a Ge atom by an incident neutron of laboratory energy E_n; $f(T)$ is the fraction of energy going into ionization, taken from averaging results of II and Ref. 5; $\sigma(E_n,T)$ is the differential elastic and inelastic scattering cross section as a function of T;

$$\int_0^{T_{\max}}\sigma(E_n,T)dT\approx\sigma_{\text{total}}(E_n)\text{ for }E_n\lesssim 3.6\text{ MeV};$$

Q_i is the energy balance for inelastic scattering to the ith excited state of a Ge isotope ($Q=0$ for elastic scattering); θ is the neutron scattering angle in the center-of-mass system; N is Avogadro's number; and A is the atomic weight of Ge. The component of energy going into atomic processes is $T[1-f(T)]$, and can be obtained by substitution of $[1-f(T)]$ for $f(T)$ in Eq. (1).

RESULTS AND DISCUSSION

The calculations of the average ionization per incident neutron and the average energy per incident neutron deposited in the atomic system are shown in Figs. 1 and 2, respectively. The calculations made at 14 MeV by Nichols[6] are also shown. As the incident neutron energy increases from 50 keV to 14 MeV, the average ionization energy deposited increases from $\sim 1\times 10^{-12}$ to $\approx 1\times 10^{-8}$ (erg/g) per (neutron/cm^2), and the energy available for displacements (nonionization) increases from $\approx 1\times 10^{-10}$ to $\approx 3\times 10^{-9}$ (erg/g) per (neutron/cm^2).

Because there are few charged-particle production cross-section data available for Ge, the actual shape of the average ionization per incident neutron as a function of neutron energy is somewhat uncertain above 3.6 MeV. The ionization for Ge (Fig. 1) seems to be about one order of magnitude smaller than for the corresponding curve for Si, for $0.3\leq E_n\leq 14$ MeV. This is largely due to the smaller energy transfer to Ge (slower recoil nuclei) and the larger Coulomb barrier against charged-particle emission in Ge. Below $\sim$0.3 MeV the rapid fluctuation of the Si cross section makes a general comparison difficult.

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[5] C. Chasman, K. W. Jones, R. A. Ristinen, and J. T. Sample, Phys. Rev. **154**, 493 (1967).

[6] D. K. Nichols, General Atomic Report No. G.A. 36, 1965 (unpublished).

Figure 2 shows that the calculations of the energy going into the Ge atomic system give a fairly good representation of the neutron energy dependence of carrier-removal data by Cleland *et al.*[7] In Fig. 2 calculations and experiment are normalized at 1 MeV. A similar proportionality was found in silicon between calculations of the energy deposited into the atomic system and carrier-removal measurements with monoenergetic neutrons.[3,8] Therefore, the neutron energy dependence of the electrical properties of neutron-irradiated Si and Ge apparently can be predicted by this type of calculation over a range of about two orders of magnitude in neutron energy. This is apparently true even though for silicon in this neutron energy range the differential scattering cross section fluctuates widely.

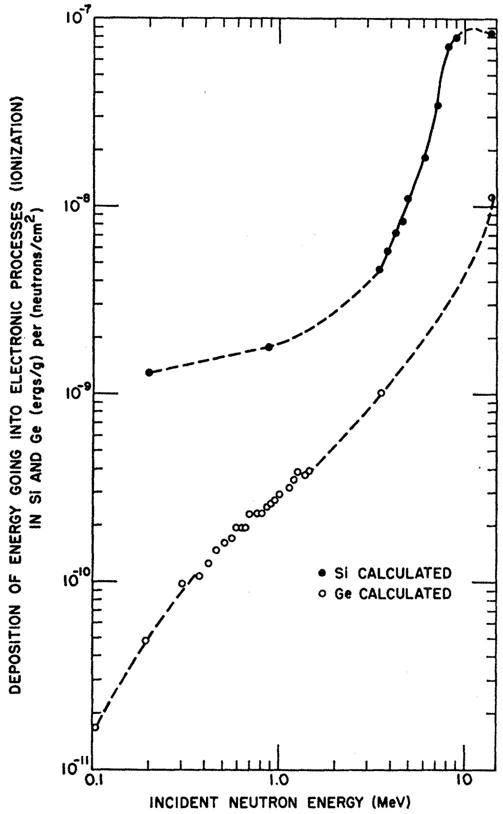

FIG. 1. Average energy deposited in Ge as ionization per incident neutron [(erg/g) per (neutron/cm²)]. The calculation at 14 MeV is taken from Ref. 6. The results for Si from Ref. 3 are shown for comparison.

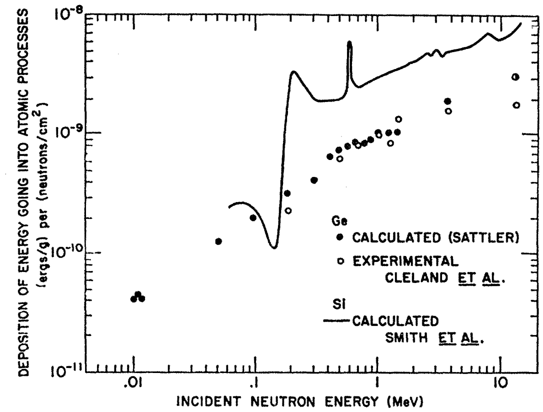

FIG. 2. Average energy deposited in Ge per incident neutron [(erg/g) per (neutron/cm²)] that does not go into ionization. Carrier-removal data are taken from Ref. 7 and normalized at 1 MeV. Shown for comparison are the calculations for Si from E. C. Smith *et al.* (Ref. 8) which are in general agreement with Ref. 3 but more detailed in the keV region. An estimate at 14 MeV taken from Ref. 6 is included.

The average energy going into the atomic system for Ge is about a factor of 2 to 3 smaller than that for Si in the energy range of 600 keV$\leq E_n \leq$14 MeV. This is about what one would expect from relative energy transfer and cross sections. For energies below ~300 keV the fluctuation of the Si cross section causes a corresponding fluctuation in the ratio of the quantity $T[1-f(T)]$ of Si to that of Ge.

$$\frac{T[1-f(T)]_{\mathrm{Ge}}}{T[1-f(T)]_{\mathrm{Si}}} \approx \tfrac{1}{10} \quad \text{at } E_n \approx 200\ \text{keV}$$

and

$$\frac{T[1-f(T)]_{\mathrm{Ge}}}{T[1-f(T)]_{\mathrm{Si}}} \approx 2.5 \quad \text{at } E_n \approx 150\ \text{keV}.$$

Now that the neutron energy dependence of permanent damage has been studied for Si and Ge in some detail, the energy deposited into the atomic system per carrier removed can be calculated for each semiconductor and compared. Since the calculated points for both Si and Ge give the shape of the experimental curve, the energy going into the atomic system necessary to remove a carrier should be neutron-energy-independent. At 1 MeV the energy going into the atomic system necessary to remove a carrier is $\sim 0.5\times10^{-9}$ erg/carrier for Ge and $\sim 1.0\times10^{-9}$ ergs/carrier for Si. These results were obtained from the data points,[7] calculations for Si,[3] and the present work on Ge. Both Si and Ge samples were float-zone *n* type, with carrier concentrations of 10^{13} carriers/cm³. It is found that the energy/carrier for Si computed from III and Cleland's measurements is the same at 1 and 14 MeV.[8]

If the number of displacements is proportional to the carriers removed, and the displacement thresholds E_d are about the same for Si and Ge, then the energy

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[7] J. W. Cleland, R. F. Bass, and J. H. Crawford, Jr., *Radiation Damage in Semiconductors* (Dunod Cie, Paris, 1965), p. 401.

[8] The energy per carrier for Si computed from the work of E. C. Smith *et al.* [IEEE Trans. Nucl. Sci. **NS-13**, 11 (1966)] and Cleland's measurements is ~25% lower at 1 MeV and ~50% higher at 14 MeV than those found in the present investigation. A calculation by H. J. Stein [J. Appl. Phys. **38**, 204 (1967)] is ~30% higher at 14 MeV. The point at 14 MeV is very difficult to calculate, however, because of the many channels available to neutron-induced reactions.

necessary to remove a carrier should also be the same for Si and Ge provided the electrical effects of the displacements are similar. The results suggest that this conclusion is approximately correct because we find (energy/carrier removal)$_{\mathrm{Si}}$/(energy/carrier removal)$_{\mathrm{Ge}}\approx 2$. The reason the ratio is not unity may be explained by uncertainties in the four quantities for Si and Ge from which this ratio was obtained. These uncertainties arise in the neutron cross-section measurements, in the carrier-removal measurements, in the exact meaning (and value) of E_d for neutron irradiation, and in the different structural and electronic nature of defects. Comparison is also difficult because near 1 MeV the Si total cross section fluctuates by a factor of 2 for larger and smaller neutron energies, and the energy spread of the "mono-energetic" neutrons at 1 MeV could influence this ratio.

Experimental results[9–11] indicate that the production of defect clusters is responsible for a large part of the electrical changes in neutron-irradiated Si and Ge. Neutron-induced disordered regions are *p*-type in Ge and intrinsic in Si. In both cases the disordered regions are surrounded by resistivity-dependent space-charge regions. For *n*-type Ge, compact *p*-*n* junctions are formed, and for *n*-type Si, diffuse intrinsic-*n*-type junctions are formed; but both of these cluster regions act similarly to block current flow in *n*-type materials. This similar behavior helps explain the similar carrier-removal results found. For *p*-type materials different results would be expected since the electrical effects of intrinsic clusters in *p*-type Si would be quite different from the electrical effects of *p*-type clusters in *p*-type Ge.

Two effects tend to make the energy imparted into the atomic system increase rather slowly with increasing neutron energy. These effects are that the differential scattering cross section becomes more forward peaked at higher neutron energies, and the fraction of the energy going into atomic processes decreases with increasing primary energy.

Many earlier calculations of the number of atoms displaced treated the total energy of the primary as the energy going into atomic processes neglecting, therefore, the effects of ionization.[12] In instances where the number of displacements are small, e.g., for heavy primaries $\sim$100 eV, the total primary energy and the energy going into atomic processes are about the same; but for primaries with energy $\gtrsim$1 keV, realistic displacement calculations should account for the fact that energy goes into ionization and is not available for the production of damage.[13] For example, in I it was shown that $\approx$80% of the energy of the 1-MeV Si atom in Si goes into ionization and only $\approx$20% of the energy therefore is available for the production of damage.

ACKNOWLEDGMENTS

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APPENDIX: DISCUSSION OF APPROXIMATIONS

The calculations presented here for Ge are more difficult than those for Si (III) because Ge is not monoisotopic, whereas Si can be considered monoisotopic. Therefore, the neutron-induced reaction channels available to each isotope of Ge must be considered. As a result, the nuclear measurements are more difficult, and the amount of available cross-section data is much smaller than for Si.

These energy partition calculations are mostly confined to the energies imparted to the Ge recoil atom over the neutron energy range, $50 \leq E_n \leq 1500$ keV, and at 3.6 MeV. This still gives an accurate representation of the energy partition because at these energies, especially below 1500 keV, the Ge Coulomb barrier ($\sim$6.5 MeV for protons and $\sim$13.5 MeV for α particles) strongly inhibits charged-particle production. Moreover, for 64% of natural Ge (Ge^{72} and Ge^{74}) the threshold for proton production is >3.20 MeV.[14] Thus, the contribution to ionization by proton production at 3.6 MeV should be small ($\sim$10% of the total ionization and $\sim$1% of the energy going into atomic processes).

The contribution of inelastic scattering (assumed isotropic) to the energy partition was taken from the work of Smith *et al.*[15] and Barry[16] in the low-energy region, and Nishimura[17] and Kent *et al.*[18] at 3.6 MeV. Because there are so many excited states from which to scatter in each of the five Ge isotopes, only the prominent ones were tabulated, although estimates

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[9] H. J. Stein, Phys. Rev. **163**, 801 (1967).

[10] O. L. Curtis, in *Radiation Effects in Semiconductors*, edited by F. L. Vook (Plenum Press, Inc., New York, 1968), p. 331.

[11] M. Bertolotti, in *Radiation Effects in Semiconductors*, edited by F. L. Vook (Plenum Press, Inc., New York, 1968), p. 311.

[12] For example, see discussions in F. Seitz and J. S. Koehler, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1956), Vol. 2, pp. 307–402; and D. Billington and J. H. Crawford, Jr., *Radiation Damage in Solids* (Princeton University Press, Princeton, N.J., 1961), pp. 11–53.

[13] J. Lindhard, V. Nielsen, M. Scharff, and P. V. Thompsen, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **33**, No. 10 (1963).

[14] J. B. Marion, *Nuclear Data Tables* (U.S. Government Printing Office, National Academy of Sciences—National Research Council, Washington, D.C., 1960).

[15] A. B. Smith *et al.* (private communication).

[16] J. F. Barry, in Proceedings of the International Atomic Energy Agency Conference on Nuclear Data, Paris, 1966 (unpublished).

[17] K. Nishimura, J. Phys. Soc. Japan **16**, 355 (1961).

[18] D. W. Kent, S. P. Puri, S. C. Snowden, and W. P. Bucher, Phys. Rev. **125**, 331 (1962).

could be made from less prominent states from their data displays. Contributions from states having nearly equal thresholds were averaged. The error from the lack of precision in the inelastic scattering cross sections in the calculations should be $\leq 20\%$ for $E_n = 3.6$ MeV and 10% for $E_n < 1.5$ MeV. Inelastic scattering accounts for $<33\%$ of the total cross section below 1.5 MeV and 50% at 3.6 MeV. The remainder of the neutron events in the energy regions are considered to be elastic scattering, and these are rather well measured and tabulated.[15,17,18] At 14 MeV the calculation of Nichols considered both heavy recoil atoms and charged particles.[6]

Below 350 keV angular-distribution cross-section data from neutron inelastic scattering were taken from neighboring isotopes[19] and normalized to the total elastic cross section of Ge. As the angular distribution becomes more isotropic at decreasing neutron energies, these data are estimated to be accurate within 15%, $50 \leq E_n \leq 350$ keV for the energy not going into ionization. For ionization, however, the results at, say, 50 keV can be considered only as an order-of-magnitude estimate because the Ge recoil energies in this range are much lower than those in the experiments of II and Ref. 5, and the calculations represent a considerable extrapolation of the data.

As in III, we neglect the ionizing effect of emitted photons (neutron-induced), considering, in effect, device-size Ge samples. Due to the much larger Z of Ge this approximation is not as valid as for Si. The photo efficiency is $\propto Z^5$, the Compton scattering is $\propto Z$, and the pair production is $\propto Z^2$. These calculations for the average ionization produced in Ge as a function of neutron energy can then be considered as a lower limit for the ionization produced as a function of incident neutron energy. The larger γ-ray efficiency for Ge would, however, have little bearing on the energy available for permanent damage.

It is interesting to note approximate relative efficiencies for samples of Si and Ge about 1 mm^3 in volume. Although the number of γ rays produced per neutron may be small and may depend upon the environment, the external γ-ray flux can be the same order of magnitude as the neutron flux in a fission environment where thermal neutrons are prominent. γ rays can then dominate the ionization, especially for germanium. Very approximate energy deposition estimates are given in Table I.

TABLE I. γ-ray ionization deposition.

Photon energy	Ionization in Si (erg/g)	Ionization in Ge (erg/g)
100 keV	$\sim 3\times10^{-7}$	$\sim 2\times10^{-6}$
1 MeV	$\sim 5\times10^{-8}$	$\sim 2\times10^{-7}$

Finally, the arguments presented in I, II, and III—that the number of pairs produced per unit amount of energy going into atomic processes is constant and independent of the type or energy of the primary in Ge—have been reinforced by recent theoretical works by Klein.[20,21] The virtual disappearance of the Fano factor suggests that the statistics of ionization in a semiconductor may imply a more efficient process than direct electron-hole production as postulated by Van Roosbroeck.[22] In order to obtain statistics of ionization more compatible with experiment it may be necessary to consider the formation of plasmons with their subsequent decay into charge pairs. This is actually postulated by Klein. He implies that the number of plasmons created depends only upon the energy deposited into the electronic system and not on the origin of the original particle (Si atom in Si versus an electron in Si). This reduces statistics of ionization to the energy of the plasmons, about one order of magnitude larger than the band gap. On the average, the number of secondary electrons created per plasmon appears to be constant. The fact that energy per charge pair produced is about the same for He^{++} and e^- ions in Si and Ge (both particles lose virtually all their energy to the electronic system), in spite of a mass difference of a factor of $\sim$7500, is experimental support of Klein's hypotheses.

A recent experiment by Haines[23] with fission fragments shows that the ratio of the electronic energy lost in the production of δ rays to the electronic energy lost in the excitation of nearby atoms is constant (for a given material) for Be, Ni, and Au metal foils. Although the mass and energy range of the fragment are limited, $75 \lesssim E \lesssim 110$ MeV, the fact that the ratio of these two electronic processes remains constant is also encouraging and in agreement with a constant value for the energy into electronic processes that is necessary to produce one electron-hole pair.

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[19] M. D. Goldberg, V. M. May, and J. R. Stehn, Brookhaven National Laboratory Report No. 400, 2nd ed., Vol. 2, 1964 (unpublished).

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