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CROSS SECTIONS FOR ATOMIC DISPLACEMENTS IN SOLIDS BY FAST POSITRONS

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ABSTRACT

The Mott series has been used to calculate the cross section for atomic displacements produced in elastic collisions between relativistic positrons and atomic nuclei. The Kinchin and Pease displacement model was used. Several elements spanning the atomic table were treated using positron energies ranging from threshold to several tens of MeV. The results are compared with previous calculations for relativistic electrons. It is found that for the same energy and atomic number the positron cross sections are always smaller (up to a factor of 5 or more). It is also found that the McKinley-Feshbach formula which is frequently used in radiation damage analysis is even less reliable for positrons than for electrons.

INTRODUCTION

The use of energetic electrons to produce radiation damage in solids is well known [1]. Their usefulness stems from several factors: A monocromatic collimated beam can be readily obtained, they have a large penetrating ability, and it is believed that they produce a simpler type of damage than heavy particles such as neutrons or heavy ions. Since a positron is the same as an electron except that its electrical charge is positive rather than negative, one would expect a positron to have similar properties for producing displacement damage. The main reason that they have not been used lies in the difficulty in obtaining a sufficiently intense source. Since more intense positron sources are a distinct future possibility, it seems worthwhile to do some exploratory damage calculations. In this paper we present some atomic displacement calculations for fast positrons and compare them with similar quantities for fast electrons [2,3].

Positrons in the energy range of one MeV possess sufficient momentum to displace atoms from their normal lattice positions directly through near head-on collisions. To calculate the probability of such a displacement it is necessary to know the scattering cross section between a positron and an atom. The scattering of a nonrelativistic positron by the Coulomb field of a point nucleus is given by the Rutherford formula and the relativistic extension was done by Mott [4] using the Dirac theory of the positron. Since positrons that can produce recoil or knock-on damage are in the relativistic range, it is necessary to use Mott's theory. Mott has expressed the Coulomb scattering of a positron (and an electron) by a point nucleus as an infinite series of Legendre polynomials. Since that series is cumbersome to evaluate, several authors have approximated it to get simpler, more tractable expressions. The so-called McKinley-Feshbach [5] version of the Mott equation that frequently is used to calculate atomic displacement cross sections for fast electrons may also be used for fast positrons. It might be expected that the McKinley-Feshbach formula for positrons would break down for heavy elements as it does in the case of electrons. In that case it would be necessary to use the more accurate Mott series formulation.

METHOD OF CALCULATION

The method used to calculate the atomic displacement cross sections by fast positrons follows closely that of fast electrons [3,5]. The calculational procedures are outlined here.

The energy transferred to a heavy nucleus by a positron scattered through an angle θ is given by

$$T = T_m \sin^2 \theta/2 \tag{1}$$

where T_m, the maximum transferred energy which occurs for a head-on collision, is

$$T_m = 2 \frac{E}{Mc^2} (E + 2mc^2) \quad . \tag{2}$$

Here E is the kinetic energy of the positron and M is the mass of the target atom. The rest energy of the positron is $mc^2 = 0.511$ MeV.

The conventional sharp displacement threshold model has been used. It assumes that an atom can be displaced only if it receives an energy equal or greater than some threshold energy, T_d. Upon receiving such an energy, the probability that the atom is displaced is taken as unity. Furthermore, the primary displaced atom can, if sufficiently energetic, produce additional displaced atoms. The cascade model used is that of Kinchin and Pease [6] which gives the average number of displacements, ν, produced by a primary knock-on of energy T as

$$\begin{aligned} \nu(T) &= 1 & T_d < T < 2T_d \\ &= T/2T_d & T > 2T_d \quad . \end{aligned} \tag{3}$$

The total cross section (primary plus secondaries) for producing atomic displacements by a positron of energy E can be written as

$$\sigma_{tot}(E,T_d) = \int_{T_d}^{T_m} \nu(T)\, \frac{d\sigma}{dT}\, dT \tag{4}$$

while the cross section for producing primary displacements only is

$$\sigma_p(E,T_d) = \int_{T_d}^{T_m} \frac{d\sigma}{dT}\, dT \ . \tag{5}$$

In Eqs. (4) and (5) the quantity $d\sigma/dT$ is the differential scattering cross section for transferring an energy T per unit T to an atom by a positron of energy E. The above integrals can be done analytically for the McKinley-Feshbach version of $d\sigma/dT$, but numerical methods become necessary when using the Mott series. Rewriting Eq. (4) more explicitly using the results of Eq. (3) gives

$$\sigma_{tot}(E,T_d) = \frac{\pi Z^2 e^4 (1-\beta^2)}{m^2 c^4 \beta^4} \left\{ \int_{T_d/T_m}^{1} \frac{dx}{x^2} M(x,E) \right\} \qquad T_d < T_m < 2T_d \qquad (4a)$$

$$= \frac{\pi Z^2 e^4 (1-\beta^2)}{m^2 c^4 \beta^4} \left\{ \int_{T_d/T_m}^{2T_d/T_m} \frac{M(x,E)}{x^2}\, dx + \int_{2T_d/T_m}^{1} \frac{T_m}{2T_d} \frac{M(x,E)}{x}\, dx \right\} \qquad T_m > 2T_d \qquad (4b)$$

where $\beta^2 = E(E+2mc^2)/(E+mc^2)^2$. Z is the atomic number of the target nucleus, e is the electronic charge and M(x,E) is the ratio of the Mott to the Rutherford cross section. The ratio M(x,E) was calculated using the method of Doggett and Spencer [7] and the integrals evaluated by 16-point Gauss-Legendre quadrature techniques. The primary displacement cross section given by Eq. (5), when written out more explicitly, becomes identical to Eq. (4a) except that now there is no restriction on the magnitude of T_m provided it is larger than T_d.

The McKinley-Feshbach differential scattering cross section per steradian is

$$\frac{d\sigma_{McK-F}(\theta)}{d\Omega} = \frac{d\sigma_R(\theta)}{d\Omega}\left[1 - \beta^2 \sin^2\frac{\theta}{2} - \pi\alpha\beta \sin\frac{\theta}{2}\left\{1 - \sin\frac{\theta}{2}\right\}\right] , \qquad (6)$$

where

$$\frac{d\sigma_R(\theta)}{d\Omega} = \frac{Z^2 e^4 (1-\beta^2)}{m^2 c^4 \beta^4 \sin^4\frac{\theta}{2}} \qquad (7)$$

is the Rutherford differential scattering cross section per steradian. Equation (6) is an expansion of the Mott series to first order in the coupling constant $\alpha = Z/137$. It is a good approximation to the series when $\alpha \ll 1$. Inserting Eq. (6) in Eq. (5) and integrating, one gets the following result for the primary displacement cross section.

$$\sigma_p = \frac{\pi Z^2 e^4 (1-\beta^2)}{m^2 c^4 \beta^4} \left[\left(\frac{T_m}{T_d} - 1 \right) - \beta^2 \ln \frac{T_m}{T_d} - \pi\alpha\beta \left\{ 2 \left[\left(\frac{T_m}{T_d} \right)^{1/2} - 1 \right] - \ln \frac{T_m}{T_d} \right] \right. . \tag{8}$$

Equations (6) and (8) also hold for electrons provided the sign of the term linear in the coupling constant α is changed from negative to positive. The range of validity of Eq. (8) will be discussed in the next section.

RESULTS AND DISCUSSION

The Mott series was evaluated using the computer code of Doggett and Spencer [7] taking 36 terms in the Legendre sums. For those cases of overlap the present results, as expected, are in excellent agreement with theirs and therefore their comments on the accuracy of the method apply here also. They have made several comparisons with other calculations and find good agreement. It should be pointed out that the present calculations were made assuming a point nucleus. At ultra high positron energies and large scattering angles this assumption becomes less valid because of nuclear size effects [4].

All of the integrations were performed using 16 point Gauss-Legendre quadrature techniques. The integration routine was checked by integrating the McKinley-Feshbach version of the Mott series numerically and comparing that with the analytical result. Excellent agreement was found.

Figure 1 shows the primary and total displacement cross sections for gold calculated using the Mott series and the McKinley-Feshbach approximation. It is seen that the latter method significantly underestimates the displacement cross sections which is not unexpected since for gold $Z = 79$ and the condition $Z/137 \ll 1$ is unfullfilled.

The primary displacement cross section using Mott and McKinley-Feshbach [Eq. (6)] scattering is shown as a ratio in Fig. 2. It is seen that for the case of uranium the McKinley-Feshbach formula may underpredict the primary displacement cross section by a factor of five or more and, of the four solids considered, it is a good approximation to the Mott series only for the relatively low Z case of copper.

Figure 3 gives the ratio of Mott to McKinley-Feshbach [Eq. (6)] scattering as a function of the positron scattering angle for uranium, gold, and silver. It is noted that the McKinley-Feshbach approximation becomes progressively poorer with increasing positron energy and with increasing atomic number. For uranium the ratio actually diverges near a scattering angle of 100 degrees. This says that the McKinley-Feshbach scattering goes to zero, a result that can be seen by examining Eq. (6). In fact Eq. (6) can become negative which leads to nonsensical predictions.

Figure 4 shows the ratio of the calculated atomic displacement cross sections of positrons to that of electrons as a function of projectile energy for four different solids. It is seen that the ratio is less than unity at all energy and for all of the cases studied. The deviation from unity is least for the relatively low Z case of aluminum and greatest for the highest Z case of gold. Although Fig. 4 was calculated using the Mott scattering series, differences between positrons and electrons are already present in the McKinley-Feshbach formula as seen in Eq. (8). The prediction that positrons cause less damage than electrons may be of relevance in studies of electron and positron channeling radiation.[8]

The present work has treated recoil or knock-on damage produced by positrons. It has not considered, for instance, damage arising through ionization that might occur in certain insulators. Knowing the cross section for recoil damage one can immediately evaluate the expected damage for a given irradiation condition. It may be mentioned that although positrons are unstable and will decay rather quickly (10^{-10} sec), their lifetimes are long compared to the positron slowing-down time. Thus, the typical positron decays after it has effectively come to rest in the solid. Finally, it should be mentioned that positron induced damage may also arise in a somewhat different context, from pair production arising from high energy gamma ray bombardment. This type of damage was briefly mentioned several years ago.[8]

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FIGURE CAPTIONS

Fig. 1. Comparison of the displacement cross sections computed from the Mott series and the McKinley-Feshbach formula for gold vs positron energy.

Fig. 2. Ratio of the primary displacement cross section computed from the Mott series to that of the McKinley-Feshbach formula for uranium, gold, silver, and copper vs positron energy.

Fig. 3. The ratio of Mott to McKinley-Feshbach scattering vs positron scattering angle for uranium, gold, and silver.

Fig. 4. Ratio of atomic displacement cross sections of positrons to that of electrons vs projectile energy.

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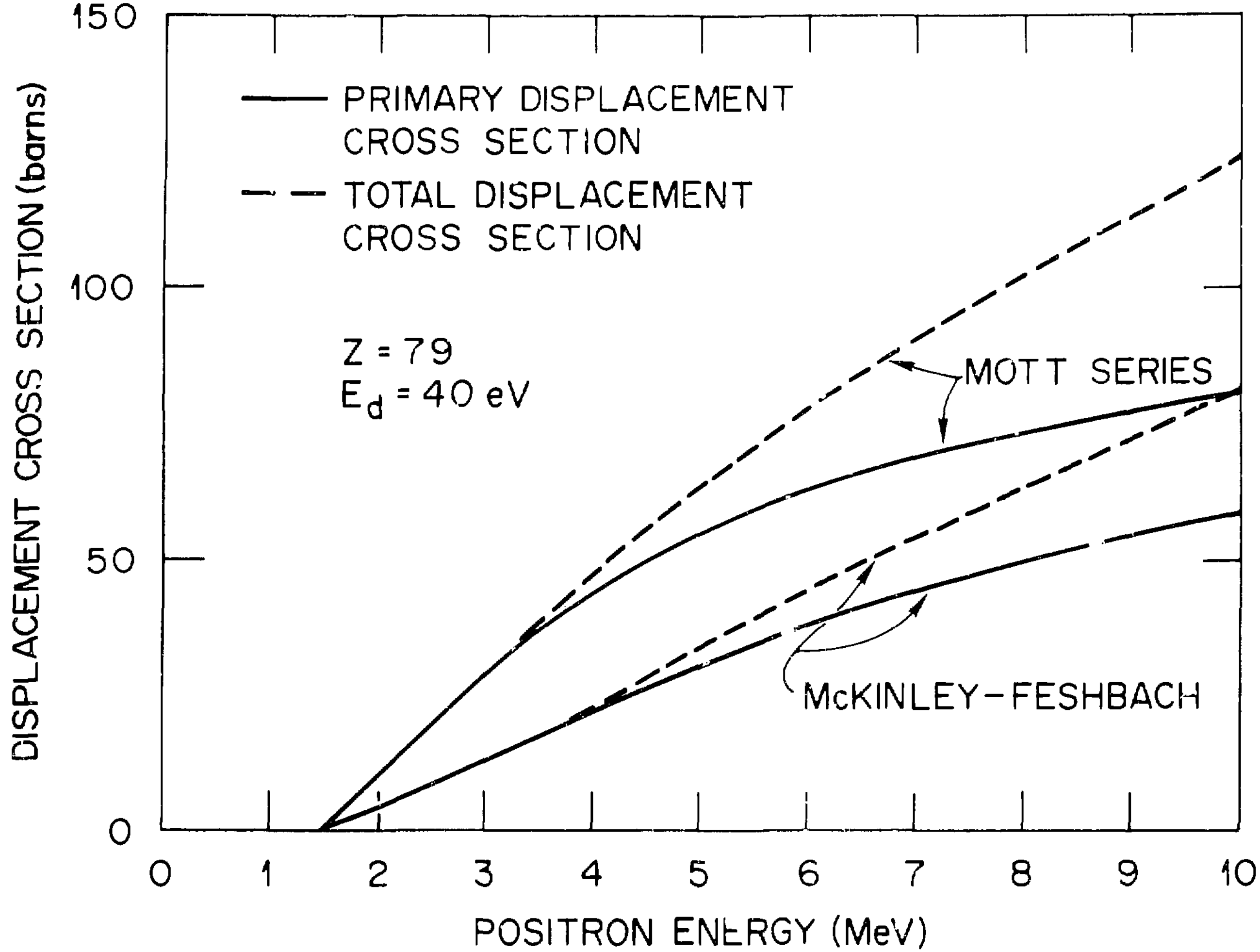
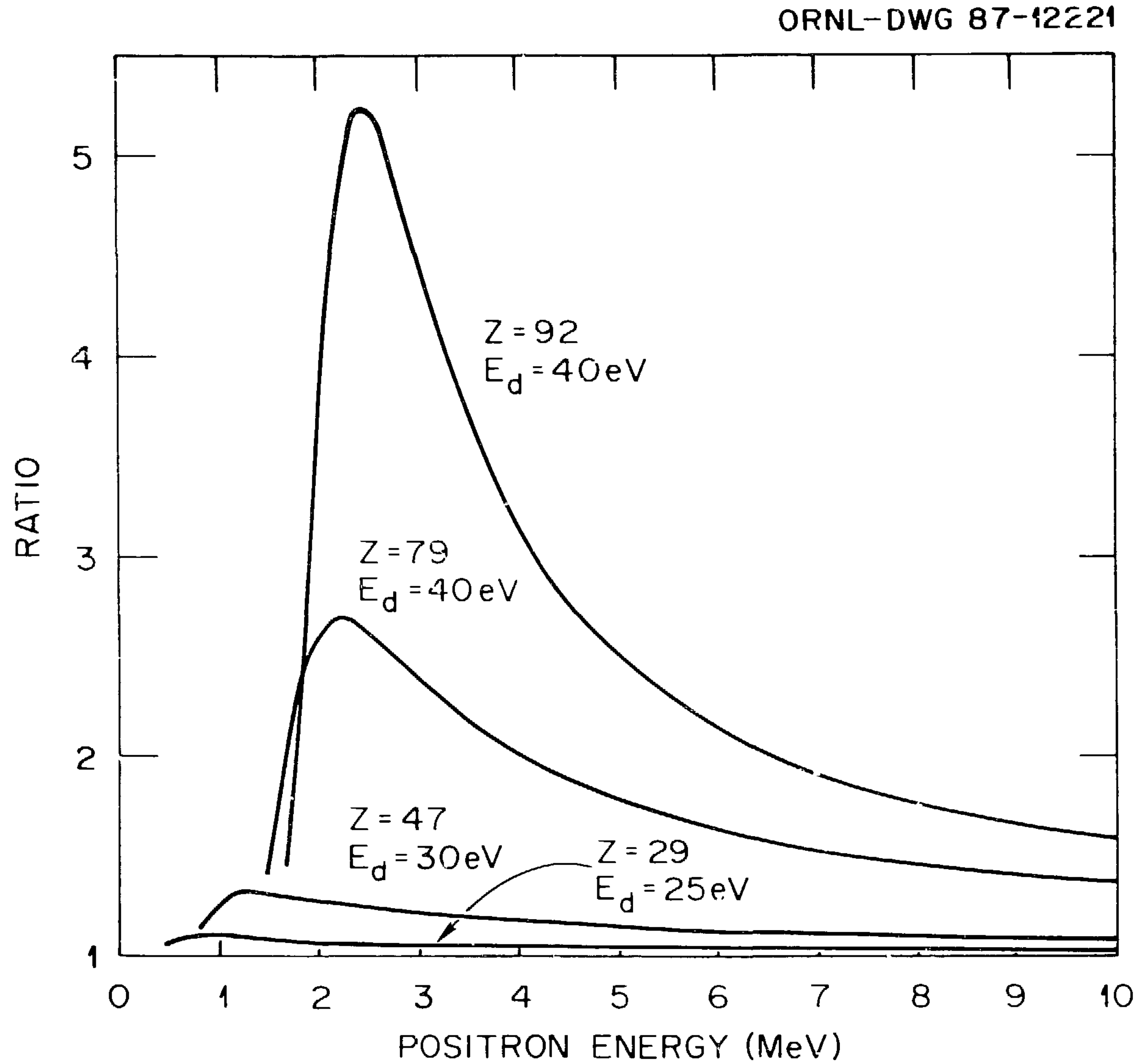


Comparison of the Displacement Cross Sections Computed from the Mott Series and the McKinley-Feshbach Formula for Gold vs. Positron Energy

Fig. 1



Ratio of the Primary Displacement Cross Section Computed from the Mott Series to that of the McKinley-Feshbach Formula for Uranium, Gold, Silver, and Copper vs. Positron Energy.

Fig. 2

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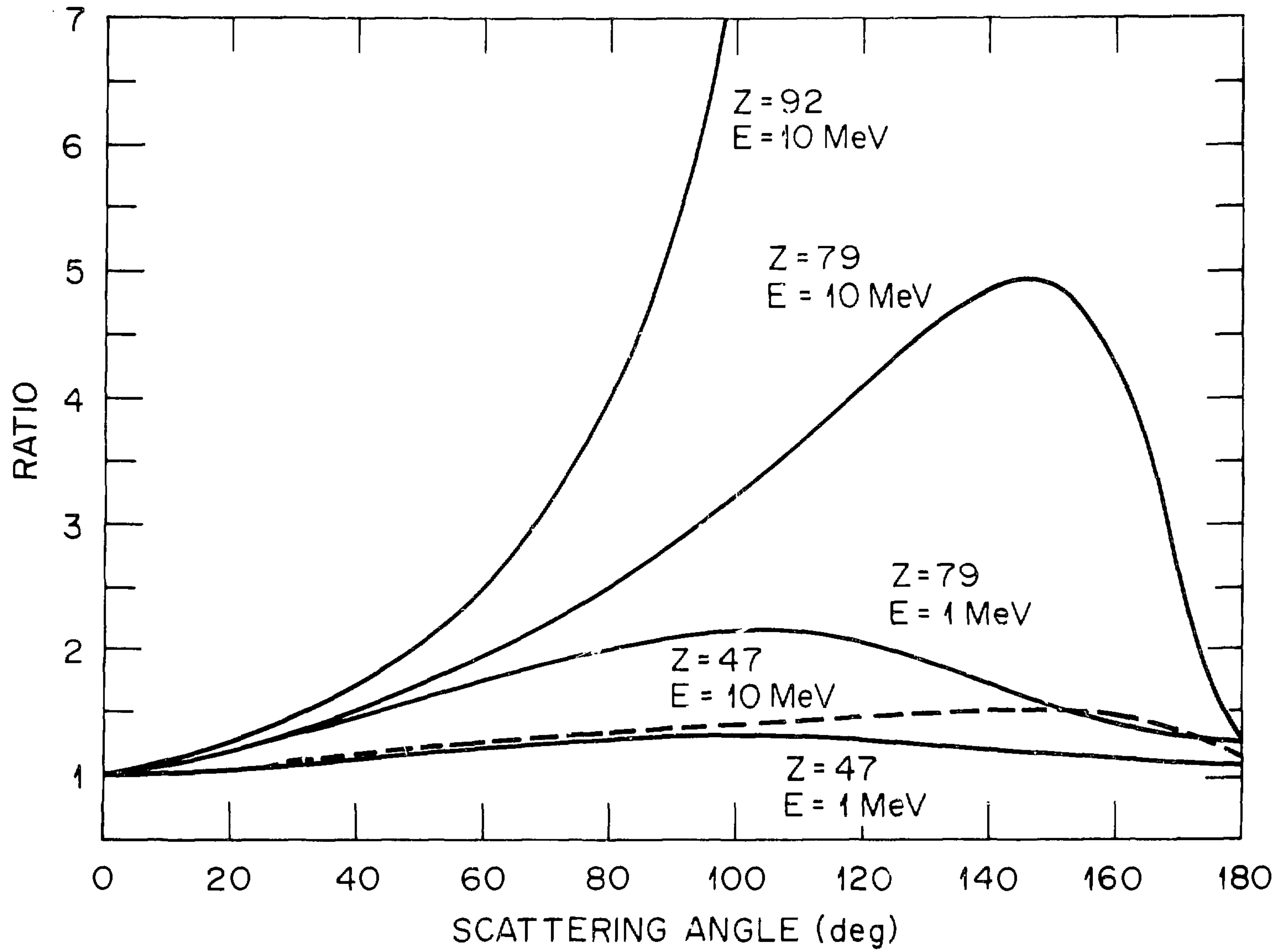
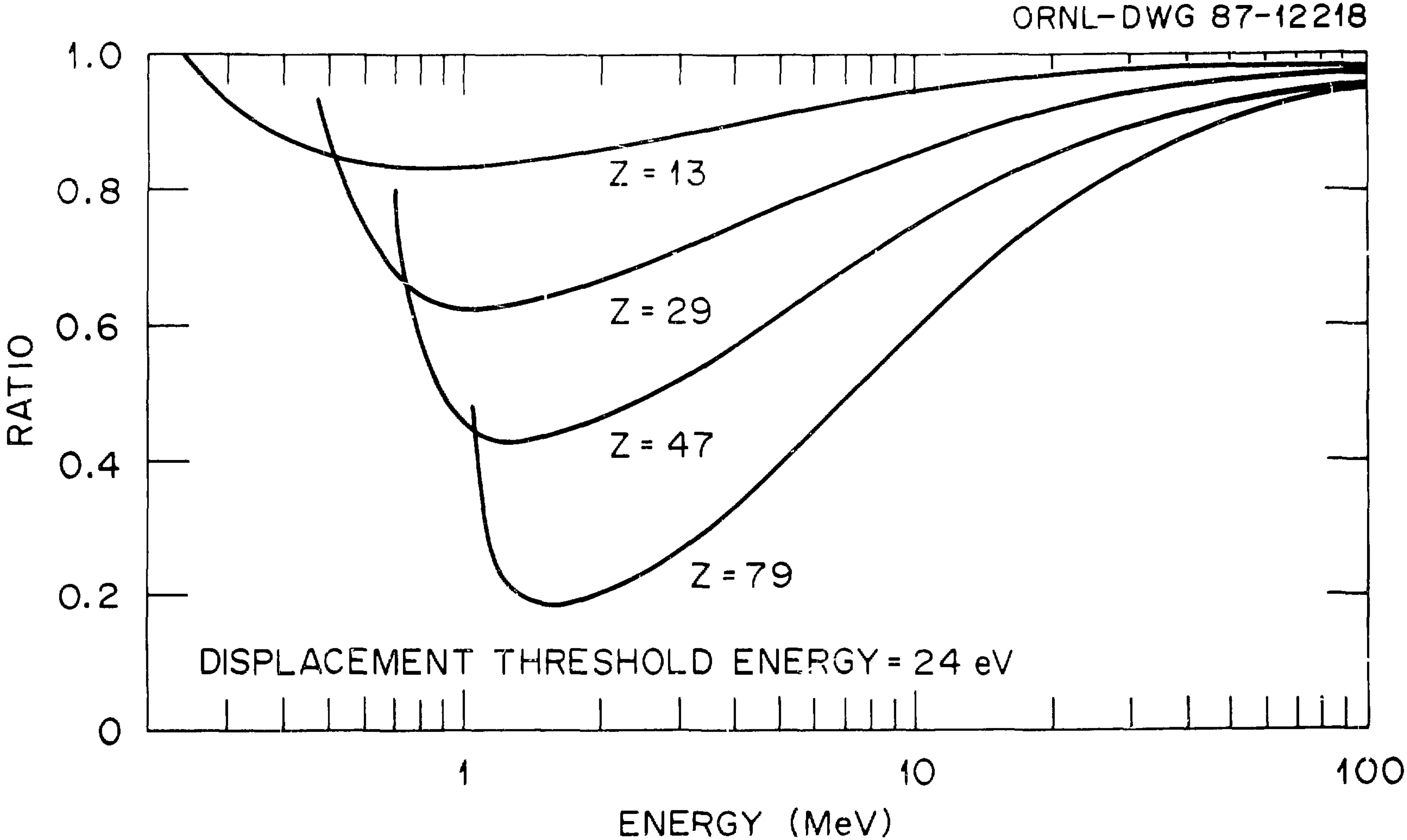


The Ratio of Mott to McKinley–Feshbach Scattering vs. Positron Scattering Angle for Uranium, Gold, and Silver.

Fig. 3



Ratio of Atomic Displacement Cross Sections of Positrons to that of Electrons vs. Projectile Energy.

Fig. 4