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Displacement Damage Caused by Gamma-rays and Neutrons on Au and Se

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Abstract

This report documents theoretical calculations of displacement damage produced by gamma rays and neutrons on various materials. The average energy of the gamma rays was 1.24 MeV and 1.0 MeV for the neutrons. The fluence of the gamma rays was $1.2 \times 10^{14} \text{ } \gamma/\text{cm}^2$, for the neutrons it was $1.0 \times 10^{12} \text{ n/cm}^2$. The initial materials of interest were Au and Se. The total doses of the gamma ray exposures were in the 100 kRad range for both elements. An equivalent electron fluence was approximated to be the same as the gamma ray fluence over one gamma ray attenuation length in both materials and at the same 1.24 MeV energy. The maximum recoil energy of the Au and Se for these electrons was calculated relativistically to be 29 and 72 eV respectively. The relativistic McKinley and Feshbach theory for the atomic recoil cross sections produced by the electrons were in the 10s of mbarn range and an upper limit for the concentration of Frenkel pairs for the gamma ray exposures for both elements was in the ppb range. The Robinson Energy Partitioning Theory for non-ionizing energy loss (NIEL) of ions in solids was used to calculate the concentration of Frenkel pairs produced by the 1 MeV neutrons, and this concentration was also in the ppb range for both Au and Se. Low damage levels like this can have effects on minority carrier recombination in semiconductors, but are not expected to have any effect on metals like Au, or metalloids such as Se.

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FIGURES

Figure 1 Calculation of Frenkel pair concentrations and displacements per atom dpa made by 1 MeV neutrons at a fluence of $1.e12 \text{ n/cm}^2$ in Au (a) and Se (b). The key parameters use white lettering in black backgrounds. 11

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1. INTRODUCTION

At the request of C. Apblett (org. 02546) theoretical calculations have been made to estimate the degree of displacement damage, i.e. the production of vacancy-interstitial Frenkel pairs, that could be produced by MeV-energy neutrons and gamma rays when exposed to solid materials. The average energy of the gamma rays was 1.24 MeV and 1.0 MeV for the neutrons. The fluences of the gamma rays was $1.2 \times 10^{14} \text{ } \gamma/\text{cm}^2$, for the neutrons it was $1.0 \times 10^{12} \text{ n/cm}^2$. The initial materials of interest were Au and Se.

2. GAMMA RAY EXPOSURES

2.1 Doses

The dose of radiation produced by gamma rays is expressed in units of Rads, where 1 Rad=100 ergs/gm. To calculate dose the following equations are used:

$$dE / dV = E_{\gamma} dN / dx \cdot 1 / A \quad (2.1)$$

$$N = N_o \exp(-\mu x) \quad (2.2)$$

$$dN / dx = N_o \mu \exp(-\mu x) \approx N_o \mu \quad (2.3)$$

where μ is the gamma ray absorption coefficient and N_o is the incident number of gammas in the beam that hits the sample over an area A, and

E_{γ} is the energy of the gamma, with $1.0 \text{ MeV} = 1.6 \times 10^{-6} \text{ ergs}$.

The energy distribution of interest was given by the following Table.

| Average Gamma Energy (MeV) | Energy Bin (MeV) | gammas/sec/MeV | σ |
|----------------------------|------------------|----------------|----------|
| 7.50E-02 | 1.00E-01 | 3.15E+05 | 3.13E+04 |
| 1.50E-01 | 2.00E-01 | 4.48E+05 | 2.58E+04 |
| 2.50E-01 | 3.00E-01 | 1.20E+06 | 4.25E+04 |
| 3.50E-01 | 4.00E-01 | 1.74E+06 | 5.12E+04 |
| 5.00E-01 | 6.00E-01 | 4.23E+06 | 5.63E+04 |
| 7.00E-01 | 8.00E-01 | 4.15E+06 | 5.48E+04 |
| 9.00E-01 | 1.00E+00 | 1.10E+06 | 2.82E+04 |
| 1.17E+00 | 1.33E+00 | 2.62E+05 | 1.08E+04 |
| 1.50E+00 | 1.66E+00 | 2.41E+05 | 1.03E+04 |
| 1.83E+00 | 2.00E+00 | 1.15E+05 | 7.01E+03 |
| 2.25E+00 | 2.50E+00 | 8.97E+04 | 5.09E+03 |
| 2.75E+00 | 3.00E+00 | 1.87E+06 | 2.32E+04 |

Table 1. The energy distribution of gamma rays

The gamma fluence of interest is calculated as $1.2 \times 10^{14} \pm 2.44 \times 10^{12}$ g/cm². The average gamma energy is 1.24 MeV.

To convert this fluence and energy to Rads, equation 2.1 needs to be slightly modified:

$$dE / dm = dE / dV \cdot dV / dm = dE / dV \cdot 1 / \rho \quad (2.4)$$

Where ρ is the mass density. Combining equations 2.1-2.4 we obtain:

$$dE / dm = E_{\gamma} (N_o / A) (\mu / \rho) \quad (2.5)$$

Where N_o/A is just the fluence of gamma rays onto the sample, μ / ρ is the usual mass attenuation coefficient.

For 1.24 MeV gamma rays, $E_{\gamma} = 2.0 \times 10^{-6}$ ergs. The dose to the two materials of interest, Au and Se, can now be calculated with equation 2.5.

| Element | μ/ρ cm ² /gm | ρ gm/cm ³ | $1/\mu$ cm | AD atoms in $1/\mu$ # atoms/cm ² | dE/dm (ergs/gm) ergs/gm | Dose Rads |
|---------|-----------------------------------|------------------------------|---------------|--|----------------------------|--------------|
| Au | 0.058 | 19.3 | 0.89 | 5.27131E+22 | 1.38E+07 | 1.38E+05 |
| Se | 0.05 | 4.8 | 4.17 | 1.52481E+23 | 1.19E+07 | 1.19E+05 |

Table 2. Dose of 1.2×10^{14} - 1.24 MeV gamma rays/cm² on Au and Se.

2.2 Atomic Displacements

Calculating the concentration of atomic displacements, i.e. Frenkel pairs created by these doses of gamma rays in Au and Se is very complicated if done rigorously. Gamma rays in the MeV energy range mainly interact with electrons in the sample through Compton scattering. These Compton electrons are the source of atomic displacements, not the gamma rays. The calculation should then involve the conversion of the gamma ray fluence to an electron fluence where the electrons would have an energy distribution given by the Compton scattering cross sections. This is beyond the scope of this short report.

We will instead assume that over one absorption length or $1/\mu$ given in Table 2 for Au and Se, that all of the 1.24 MeV gamma rays are converted to 1.24 MeV electrons. We will now calculate the number of atomic displacements that this fluence of electrons can make inside this absorption length.

First we need to calculate the maximum energy of the target atoms made by these 1.24 MeV electrons. The energy of these electrons is much greater than their rest mass of .511 MeV, and therefore we have to use equations that are relativistic.

$$T_{max} = \frac{2p_o^2}{M} = \frac{2(\gamma m v_o)^2}{M} = 2 \frac{m}{M} \gamma^2 \beta^2 m c^2 \quad (2.6)$$

Where T_{max} is the maximum energy the electron can transfer to a target atom, i.e. a head-on collisions, and

$$\beta = v / c \quad (2.7)$$

$$\gamma = \frac{1}{\sqrt{1 - \beta^2}} \quad (2.8)$$

m is the mass of the electron, M the mass of the target atoms, v the electron velocity and c the speed of light.

| Element | m | Z | M | T-max | T-min | σ -McF |
|---------|----------|----|-----|-------|-------|---------------|
| | amu | | amu | eV | eV | barns |
| Au | 0.000545 | 79 | 197 | 29 | 14.5 | 62 |
| Se | 0.000545 | 34 | 79 | 72 | 36 | 11.5 |

Table 3. Maximum recoil energy of Au and Se by 1.24 MeV electrons

Now it is not even clear whether 29 eV is enough energy to create a Frenkel pair in Au, but we assume that it is. One thing that is clear is that this calculation will be for a worst case in that it will overestimate displaced atom concentration. This is because most of the Compton electrons will have energies less than 1.24 MeV, and the energy of the Au and Se atoms recoiled will be less than the T_{max} values given in Table 3.

We need to know the cross section for the electrons to recoil the target atoms, at fairly high energy, and if we assume that it takes at least half of the T_{\max} recoil energies to create a vacancy then $T_{\min}=0.5T_{\max}$. We can then use the relativistic and quantum mechanical cross section derived by McKinley and Feshbach in 1948 (1) to estimate this cross section.

$$\sigma_{McF} = \pi \left(\frac{Ze^2}{mc^2} \right)^2 \frac{1}{\beta^4 \gamma^2} \left[\left(\frac{T_{\max}}{T_{\min}} - 1 \right) - \beta^2 \ln \left(\frac{T_{\max}}{T_{\min}} \right) + \pi \alpha \beta \left\{ 2 \left[\left(\frac{T_{\max}}{T_{\min}} \right)^{1/2} - 1 \right] - \ln \left(\frac{T_{\max}}{T_{\min}} \right) \right\} \right] \quad (2.9)$$

Where Z is the atomic number of the target atoms, e is the fundamental electron charge (in this treatment we use $e^2=1.44$ MeV fm) and α is the fine structure constant = $1/137$. The recoil cross sections for 1.24 MeV electrons on Au and Se are listed in Table 3 above.

The concentration of Frenkel pairs per unit volume C_{FP} can be expressed as:

$$C_{FP} = \Phi_e \sigma_{McF} C_a \quad (2.10)$$

where Φ_e is the fluence of electrons ($1.24e14$ e/cm²), σ_{McF} is the recoil cross section given in Eq. 2.9, and C_a is the concentration of target atoms (#/cm³). The following table summarizes the calculation.

| Element | m | Z | M | T-max | T-min | σ -McF | Ca | C-FP | displacements |
|---------|----------|----|-----|-------|-------|---------------|-------------|-------------|---------------|
| | amu | | amu | eV | eV | barns | # atoms/cm3 | FPs/cm3 | per atom |
| | | | | | | | | | dpa |
| Au | 0.000545 | 79 | 197 | 29 | 14.5 | 62 | 5.87817E+22 | 4.51914E+14 | 7.688E-09 |
| Se | 0.000545 | 34 | 79 | 72 | 36 | 11.5 | 3.64557E+22 | 5.19858E+13 | 1.426E-09 |

Table 4. Calculation of atomic displacements produced by 1.2e14 1.24-MeV electrons in the gamma ray absorption length of Au and Se using the McKinley and Feshbach theory.

As mentioned above the assumptions used in this calculation overestimates the displacement damage caused by the gamma rays, but nevertheless it is extremely low, in the ppb range.

3. NEUTRON EXPOSURES

A excel program, DEDX6Rob7.xls that has been used for years to calculate the 1 MeV equivalent neutron fluences for ion beams in the IBL was used to calculate the displacements made by $1.e12$ n/cm² in Au and Se. To use the program, however, we must assume their energy to be 1 MeV in order to use the neutron stopping cross section of 95 mbarn-MeV.

This code is based on the Robinson Energy Partitioning Theory for non-ionizing energy loss (NIEL) of ions in solids [2,3].

The code is really designed to calculate the 1 MeV equivalent neutron fluence for a given ion fluence, and so in this instance we are doing the reverse. That is, we change the ion fluence, e.g.

a 1 MeV Au beam into Au, or similar for Se, to get $1.e12 \text{ n/cm}^2$ and read off the Frenkel pair concentration and displacements per atom – dpa. The input and output of the code are shown for Au and Se in the next two figures.

| ENTER Z1,Z2s,AND E and rho(use) IN THE YELLOW CELLS | | | | | | | | | | LET is MeV/mg/cm2 | |
|---|------------|-------------|----------|-------------|-------------|---------------------|----------|---------------|--|-------------------|--|
| Target= | Au | | area= | 1 cm2 | | size= | 10000 um | | pulse time (us)= | 1 | |
| Proj. Z= | 79 | 196.967 | ions/s= | 8.8542E+10 | | 8.85E+10 ions/cm2/s | | Sn n (mbMeV)= | 95 | | |
| E1(MeV)= | 1 | Au | i(nA) | 8.50E+01 | | q= | 6 | | depth(um)= | 0.1 | |
| Tar. Z2= | Au | H | H | H | H | H | H | tot | A | | |
| compo= | 79 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 196.97 | | |
| m frac.= | 100% | 0% | 0% | 0% | 0% | 0% | 0% | 1 | 1 | | |
| rho(use)= | 19.3 | g/cm3 | calc= | 19.30 g/cm3 | | eV/eh= | 4.60 | | 25.00 | | |
| atomic conc= | 5.9E+22 | atoms/cm3 | | | | | | | | | |
| Surface | Elec | | NIEL | | range(um) | | at | | 0.1 um | | |
| Calc LET= | 2.26E-02 | LET= | 3.77E+00 | | Approx= | 22.89 | | E (MeV) = | 0.115128072 | | |
| rad/s= | 3.21E+04 | dpa/s= | 0.001745 | | EOR= | 0.13 | | LET = | 0.053943313 | | |
| eV/A= | 4.37E+00 | eV/A= | 7.27E+02 | | ions/cm2= | 88541.66667 | | Sn (mbMeV)= | 1089032475 | | |
| rads= | 3.21E-02 | dpa= | 1.74E-09 | | fp/ion/s | 0.013508766 | | n/cm2s= | 1.015E+18 | | |
| eV/mol/cm2= | 7.40E-15 | (mb(MeV)= | 1.23E+09 | | d-fraction= | 0.728664937 | | n/cm2= | 1.01E+12 | | |
| eh/cm3= | 8.41E+12 | fp/cm3= | 1.03E+14 | | FPF= | 1.16E+09 | | FPF= | 1028344472 | | |
| Damage Factor (nonionizing)= | 7284123.51 | 12965739.84 | | | | | | | Damage Factor (nonionizing)= 11463499.74 | | |

a.

| ENTER Z1,Z2s,AND E and rho(use) IN THE YELLOW CELLS | | | | | | | | | | LET is MeV/mg/cm2 | |
|---|-----------|------------|-----------|------------|-------------|---------------------|----------|---------------|---|-------------------|--|
| Target= | Au | | area= | 1 cm2 | | size= | 10000 um | | pulse time (us)= | 1 | |
| Proj. Z= | 34 | 78.960 | ions/s= | 4.1354E+11 | | 4.14E+11 ions/cm2/s | | Sn n (mbMeV)= | 95 | | |
| E1(MeV)= | 1 | Se | i(nA) | 3.97E+02 | | q= | 6 | | depth(um)= | 0.1 | |
| Tar. Z2= | Se | H | H | H | H | H | H | tot | A | | |
| compo= | 34 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 78.96 | | |
| m frac.= | 100% | 0% | 0% | 0% | 0% | 0% | 0% | 1 | 1 | | |
| rho(use)= | 4.8 | g/cm3 | calc= | 4.80 g/cm3 | | eV/eh= | 4.60 | | 25.00 | | |
| atomic conc= | 3.66E+22 | atoms/cm3 | | | | | | | | | |
| Surface | Elec | | NIEL | | range(um) | | at | | 0.1 um | | |
| Calc LET= | 2.95E-01 | LET= | 1.13E+00 | | Approx= | 7.07 | | E (MeV) = | 0.901428523 | | |
| rad/s= | 1.95E+06 | dpa/s= | 0.00098 | | EOR= | 0.90 | | LET = | 0.240353497 | | |
| eV/A= | 1.41E+01 | eV/A= | 5.42E+01 | | ions/cm2= | 413541.6667 | | Sn (mbMeV)= | 229811568.1 | | |
| rads= | 1.95E+00 | dpa= | 9.80E-10 | | fp/ion/s | 0.002304245 | | n/cm2s= | 1.00039E+18 | | |
| eV/mol/cm2= | 3.86E-14 | (mb(MeV)= | 1.48E+08 | | d-fraction= | 0.670448133 | | n/cm2= | 1.00E+12 | | |
| eh/cm3= | 1.27E+14 | fp/cm3= | 3.588E+13 | | FPF= | 8.68E+07 | | FPF= | 134629065 | | |
| Damage Factor (nonionizing)= | 875848.47 | 1559010.28 | | | | | | | Damage Factor (nonionizing)= 2419069.14 | | |

b.

Figure 1 Calculation of Frenkel pair concentrations and displacements per atom dpa made by 1 MeV neutrons at a fluence of $1.e12 \text{ n/cm}^2$ in Au (a) and Se (b). The key parameters use white lettering in black backgrounds.

In these calculations we used self ion implantation since the primary knock-on atoms (PKAs) produced by the neutrons are the target atoms themselves. The displacement energy threshold was assumed to be 25 eV. For this neutron fluence of $1.e12 \text{ n/cm}^2$, the dpa's are in the ppb range for both Au and Se.

4. CONCLUSIONS

Theoretical calculations have been made to estimate the degree of displacement damage, i.e. the production of vacancy-interstitial Frenkel pairs that could be produced by MeV-energy neutrons and gamma rays when exposed to solid materials. The average energy of the gamma rays was 1.24 MeV and 1.0 MeV for the neutrons. The fluences of the gamma rays was $1.24 \times 10^{14} \text{ } \gamma/\text{cm}^2$, and for the neutrons it was $1.0 \times 10^{12} \text{ n/cm}^2$. The initial materials of interest were Au and Se.

Minimal displacement damage is expected to be produced for both the gamma ray and neutron exposures at the above energies and fluences based on these calculations. The number of displacements per atom, or dpa, for both exposures and for both Au and Se are in the ppb range.

Low damage levels like this can have effects on minority carrier recombination in semiconductors, but are not expected to have any effect on metals like Au, or metalloids like Se.

5. REFERENCES

1. W.A. McKinley and H. Feshbach, Phys. Rev. 74 (1948) 1759.
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