Spatial Distribution of Electron-Hole Pairs Created by Photons in Detector Materials

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Outline

• **Introduction**
  - Spatial distribution of electron-hole pairs (e-h) – previous simulations
  - Calculation of e-h pair yield
  - Several issues to be addressed

• **Monte Carlo Model**

• **Production of e-h pairs**
  - Electron cascade and number distribution of e-h pairs
  - \( W \) value and *Fano* Factor

• **Spatial Distribution of Electron-Hole Pairs**
  - Conventional detailed MC method
  - Spatial distributions of electron-hole pairs (in Ge)
Introduction

Most previous simulations of e-h pairs – only consider track structure of secondary electrons created by photons to evaluate \( \frac{dE}{dx} \) [NIMA 563 (2006) 116]

Total deposited energy: 100 keV electron in CdZnTe – linear electron cascade

- e-h pair density (or number of e-h pairs) - \( \rho = \frac{1}{W} \frac{dE}{dx} \)
  
  \( W \) – mean energy required to create an electron-hole pair
Introduction


- Nonlinear electron cascade- more accurate calculations of intrinsic properties

- Nonlinearity observed in scintillators

- Several issues – detailed distribution of e-h pairs
  - e-h pair recombination
  - Nonlinear electron cascade- more accurate calculations of intrinsic properties
  - Nonlinearity observed in scintillators

E-h pair distribution by a 140 keV photon in amorphous-Si
Monte Carlo Model

- Model – interaction of photon with materials:
  - Photoelectric absorption
  - Compton scattering
  - Electron-positron pair production

- Model – detailed energy-loss mechanisms for electrons (inelastic)
  - Electron-Phonon interaction
  - Valence Band Ionization
  - Excitation of Plasmons and Decay
  - Core shell ionization (K and L-shell…..)
  - Shake-off electrons
  - Bremsstrahlung emission – energy loss
  - Band structure effects (for semiconductors)
  - Stopping criteria for electrons – 2.5 eV

- Model – elastic interaction

- Mean free path between collisions:
  \[ \lambda^{-1} = N(\sigma^{el} + \sigma^{in}) \]
Electron Cascades in Ge

- Photon energy – 50 eV ~ 2 MeV
- Number of simulations for each energy – $10^5$ (statistics)
- Band gap – 0.74 for Ge

Electron distribution in Ge

- Asymmetric
- Not perfect Gaussian distribution
- No. electrons/event = 16.8, 54.3 and 224.6 for 50, 150 and 600 eV, respectively
Electron Cascades in Ge

- Symmetric distribution
- Approximate Gaussian distribution
- No. electrons ~ 557.4 and 2893.2 for 40 and 662 keV, respectively
- Height of the distribution decreases with increasing energy
- Width of the distribution increases with increasing energy

662 keV gamma ray from $^{137}$Cs
Electron Cascades in Ge

- **W** value and Fano Factor

- **W:** For $E (> 2 \text{ keV})$, ~ 2.64 eV (exp: 2.6 – 2.9 eV)
- **F:** For $E (> 2 \text{ keV})$ 0.11 (exp: 0.09 ~ 0.195)
Electron Cascades in Several Materials

- Intrinsic resolution: \[ \Delta E_{in} = \frac{\sqrt{8 \ln(2)} WF}{E} \]

![Graph showing simulations and experiments for different materials]

- Band gap (eV)
- Energy (E)
- Simulations
- Experiments
- Ge
- SiGe
- Si
- CZT

\[ \Delta E_{in} = 2.355 \left[ \frac{0.12E_g^2 + 0.22E_g + 0.057}{E} \right]^{1/2} \]
Spatial Distribution of e-h Pairs

- Distribution of electron-hole pairs in Ge (2 keV)

- Electrons created by plasmon – along the track
- Electrons created by interband transition – at periphery of cascade volume
- There are some single electrons and holes.
- Most electrons and holes are close to each other.
- Thermalized electrons can move away from cascade volume.

40 nm
Spatial Distribution of e-h Pairs

- Distribution of electron-hole pairs in Ge (2 keV)

- Distribution of electron-hole pairs is different for different cascade (same energy)
- Density of electron-hole pairs along main path is high
- Density of electron-hole pairs at the periphery of cascade volume is low.
Spatial Distribution of e-h Pairs

- Distribution of electron-hole pairs in Ge (10 keV)

- Nonlinear electron cascade
Dynamic process of electron-hole pair creation (1 keV)
Conclusions

- A Monte Carlo code has been developed to simulate electron cascade, production of e-h pairs and their number distribution in detector materials.

- Intrinsic resolution in semiconductors follows:

\[
\frac{\Delta E_{\text{in}}}{E} = 2.355 \left[ \frac{0.12 E_g^2 + 0.22 E_g + 0.057}{E} \right]^{1/2}
\]

- Plasmon and interband transition are major mechanisms to generate e-h pairs in semiconductors.

- Spatial distribution of e-h pairs indicates that electrons created by plasmon are along the track, while electrons created by interband transition distribute at the periphery of cascade volume - nonlinear electron cascade.
Thank You
Monte Carlo Model

- Cross sections – based on the generalized oscillator strength model, a new model has been developed.
- Total cross section – within 2%-8% of experimental measurements
- Band structure effects on cross sections at low energy (<20 eV) must be calculated
First-Principles Approach

- Differential electronic scattering cross section determined by dielectric function

\[
\frac{\partial \sigma(q, \omega)}{\partial q \partial \omega} = -\frac{8\pi \Im[\varepsilon^{-1}(q, \omega)]}{q^2} \nu n
\]

- Dielectric function is a function of band energies and orbitals

\[
\varepsilon(q, \omega) = f(E_{n,k}, < r | n, k >)
\]

- Need band energies \( E_{n,k} \) and orbitals \( < r | n, k > \)
  - Use ABINIT code to get band structure - Plane wave basis set, pseudopotentials
  - Correct DFT band energies using GW method.
  - Use DFT Kohn-Sham eigenfunctions for orbitals
First-Principles Approach

- Our calculated dielectric function for silicon is similar to experiments

With differential cross section known, we can integrate over $q$, $\omega$ to find total cross section & electron mean free paths.

- Determine secondary particle (electron, hole) spectrum from plasmon decay


Experiment


Theory

Pacific Northwest National Laboratory
U.S. Department of Energy
First-Principles Approach

- Cross section – ab initio data model

- Total cross section is in reasonable agreement with that from ab initio data model.

- We will apply the ab initio data model to known and unknown materials.

- Solving the partial-wave expanded Dirac equation for the motion of the projectile in the field of the target atom

\[
\frac{d\sigma_{el}}{d\theta} = |f(\theta)|^2 + |g(\theta)|^2
\]

\[
f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} \{ (l+1)[\exp(2i\delta_{l-}) - 1] + 1[\exp(2i\delta_{l+}) - 1] \} P_l(\cos \theta)
\]

\[
g(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} \{ \exp(2i\delta_{l-}) + \exp(2i\delta_{l+}) \} P_l(\cos \theta)
\]

- DCS

\[
\sigma_{el} = \int \frac{d\sigma_{el}}{d\theta}
\]

\[\delta_i \text{ – phase shifts} \]

\[P_l(cos \theta) \text{ – Legendre polynomials} \]
Spatial Distribution

- Approach – conventional detailed MC method
  - Each simulated path of a particle – characterized by a series of states:
    \[ \{r_n, E_n, \cos \theta_n \} \]
  - Mean free path between collisions:
    \[ \lambda^{-1} = N(\sigma^{el} + \sigma^{in}) \]
  - Length \( s \) of the free path to the next collision is obtained by random sampling from the distribution:
    \[ p(s) = \lambda^{-1} \exp(-s/\lambda) \quad \Rightarrow \quad r_{n+1} = r_n + s \cos \theta_n \]
  - If elastic collision, \( \theta \) is sampled from the distribution;
  - If inelastic collision, \( \theta \) is fixed by energy and momentum conservation:
    \[ Q(Q + 2mc^2) = c^2 \left( p^2 + p'^2 - 2pp' \cos \theta \right) \]
    
    Momentum transfer – \( q=p-p' \)
    
    Recoil energy, \( Q - Q=\sqrt{(cq)^2+mc^2} - mc^2 \)
  - Azimuthal scattering angle, \( \phi \) – \( \phi = 2\pi \text{rand}() \)

- \( p(\theta) = \frac{1}{\sigma^{el}} \frac{d\sigma^{el}}{d\theta} \)

- Depends on type of inelastic collisions