



Modeling the Fine Structure in Spectra from Silicon X-Ray Detectors using Monte-Carlo Methods

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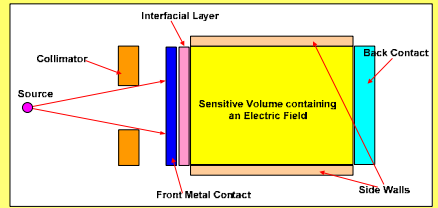
(1) Objectives

- Understand the basic processes occurring in silicon x-ray detectors.
- Predict response functions for different geometries.
- Model artifacts in energy-dispersive spectra, such as escape peaks, edge effects, contacts, "ghost" peaks.
- Suggest ways to improve the design and manufacturing of Si(Li) detectors.
- Model effects on quantitative chemical analysis using energy-dispersive x-ray detectors.

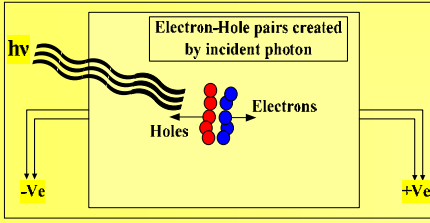
(2) Monte-Carlo Model Parameters

- Active Si(Li) volume, front contact, interfacial (dead) layer
- Rear contact, passivation side walls, charge traps
- Simple symmetric geometries – circular or square cylinders
- Hot electrons – photoelectrons and Auger electrons
- Photoelectric absorption, Rayleigh and Compton scatter
- Electron and hole carriers, lifetimes and mobilities
- Charge collection efficiency vs. depth
- Fano-factor line broadening
- Electron and photon losses

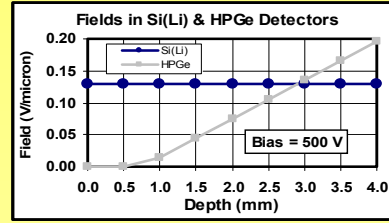
(3) Simplified Si(Li) Detector Model



(4) Electron-Hole Pair Creation



(5) Electric Fields in Semiconductor Detectors

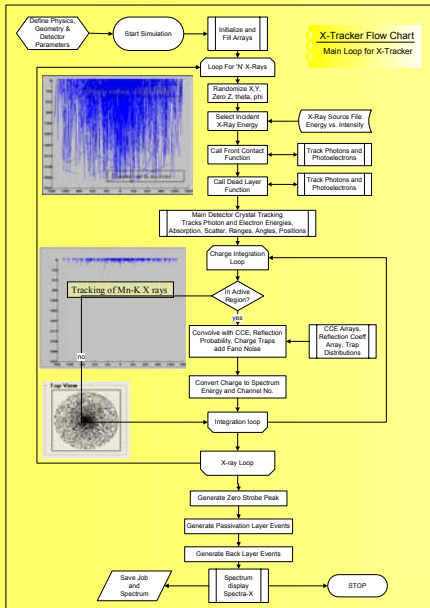


(6) Ramo Theorem and Hecht Equation

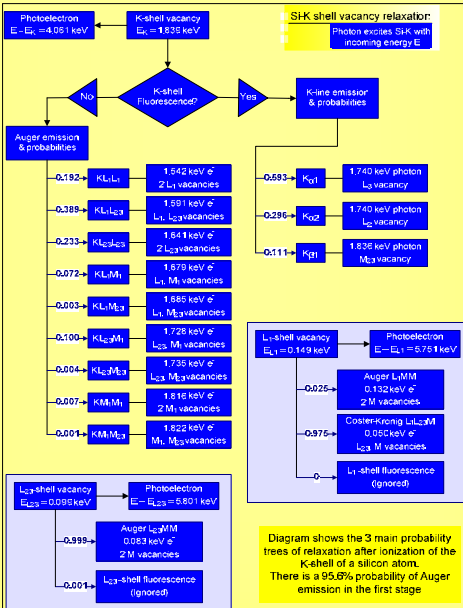
• Si(Li) detectors have uniform field gradient
 • Incoming photon interacts with Si & generates charge clouds
 • Motion occurs as per Schockley-Ramo Theorem:
 $dQ^* = -eN_0/L * (dx_e + dx_h)$
 • Charge traps occur from impurities or crystal defects
 • Charge Collection Efficiency (CCE) then obeys Hecht equation over depth of detector:

$$Q^* = \frac{eN_0}{L} \cdot \left[v_h \tau_h \left(1 - \exp\left[-\frac{x_e}{v_h \tau_h}\right] \right) \right] + \left[v_e \tau_e \left(1 - \exp\left[-\frac{x_h - L}{v_e \tau_e}\right] \right) \right]$$

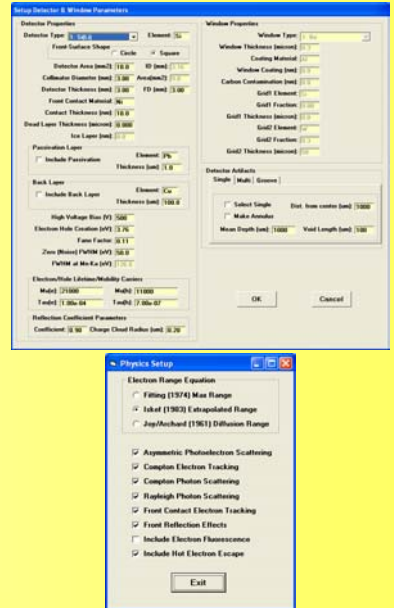
(7) Main Monte-Carlo Program Flow Chart



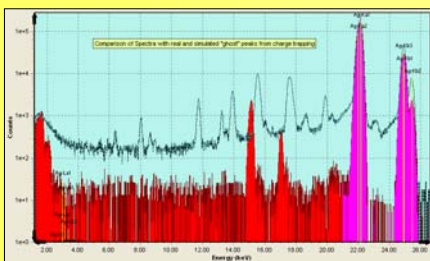
(8) Ionization Relaxation of K Shell of Si Atom



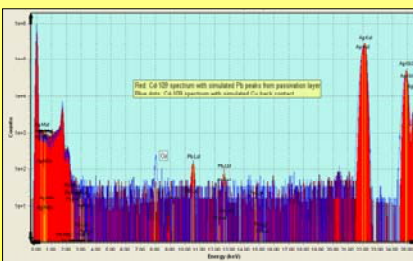
(9) Setup Screens for Monte-Carlo Model



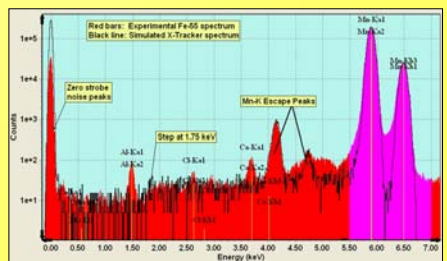
(10) "Ghost" Peaks – Vary with Bias Voltage



(11) Simulated Passivation & Contact Peaks



(12) Compare Real & Simulated Fe-55 Spectra



(13) Conclusions

- Have successfully modeled performance of Si(Li) detectors below 10 keV, and to a lesser extent for higher-energy spectra.
- Good fits to background from zero to main peaks for Fe-55 spectra.
- Able to simulate detector artifacts such as escape peaks, passivation layer, back contacts, "ghost" peaks from charge traps, etc.
- Reflection coefficient and interfacial layers included in the model.
- In the future we need to improve peak tails & include radiative Auger peaks for low-energy spectra, and background fit for high-energy spectra.

(14) References

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(15) Acknowledgements

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