# Microdosimetry and Spectral Emissions of Metal Tritide Particles

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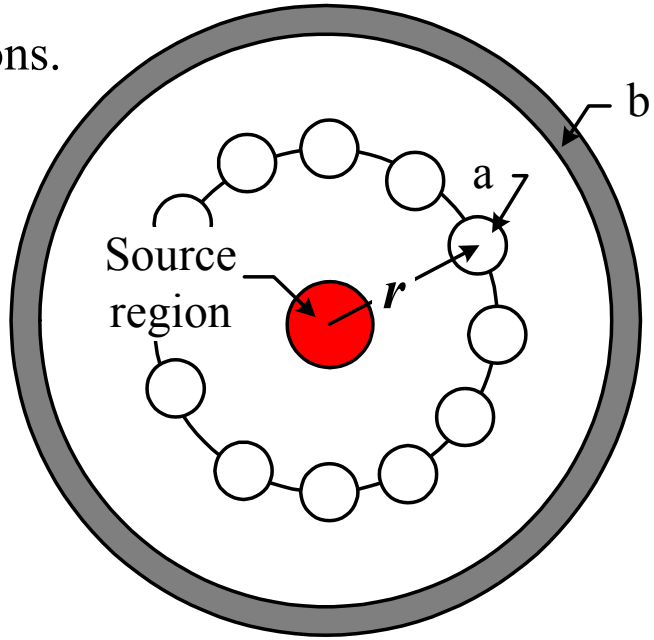
# Methodology

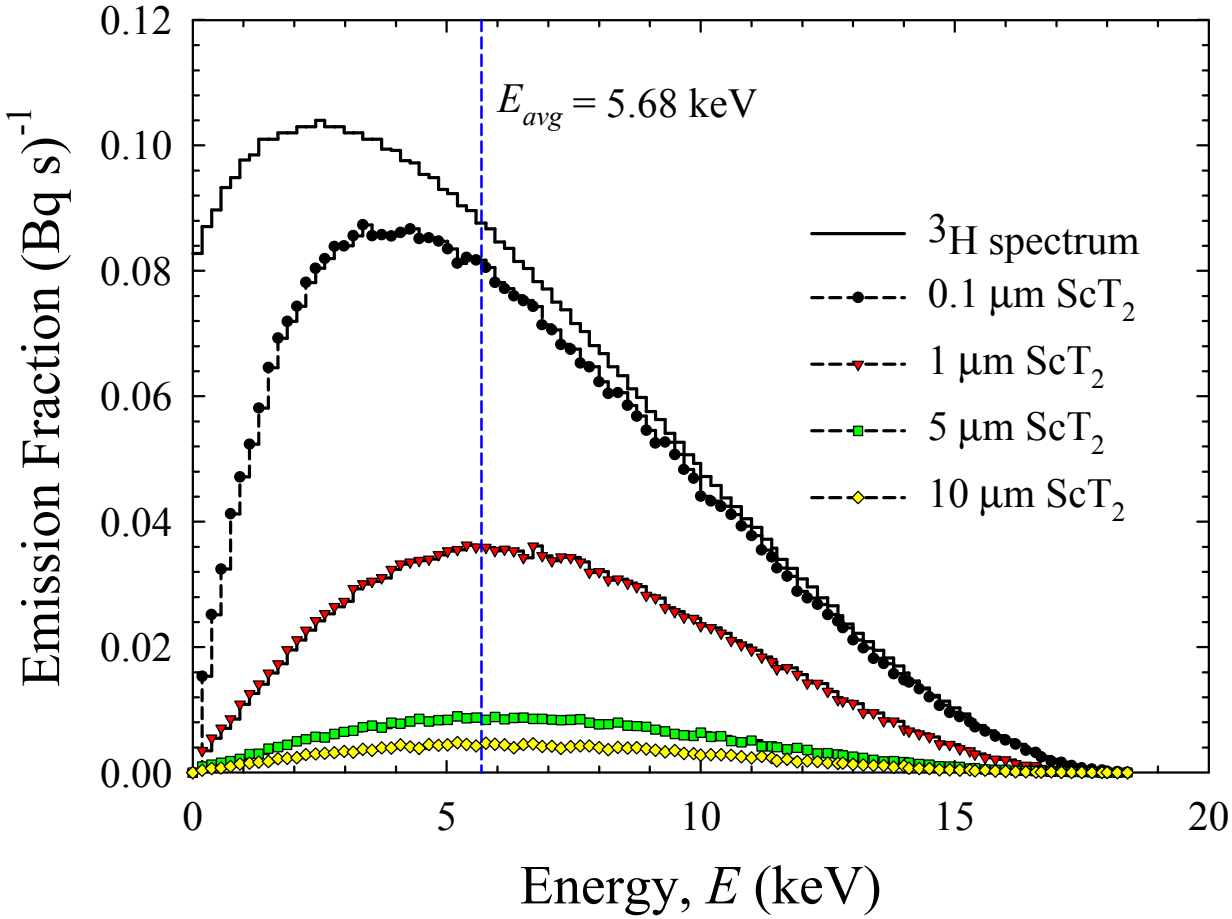
- Electrons and photons transported through the metal tritide and surrounding soft tissue using the PENELOPE (Salvat *et al.* 1999) Monte Carlo radiation transport code.
  - 100 eV cutoff energy for electrons and positrons.
  - 1 keV cutoff energy for photons.




- Absorbed dose and fluence calculations compare favorably to the EGS4, ETRAN, and the ITS3 code systems (Sempau *et al.* 1997).
- Microdosimetric quantities comparable to those computed using the PITS analog Monte Carlo code system (Stewart and Wilson 2000, unpublished).
  - Site sizes greater than about 200 to 500 nm.

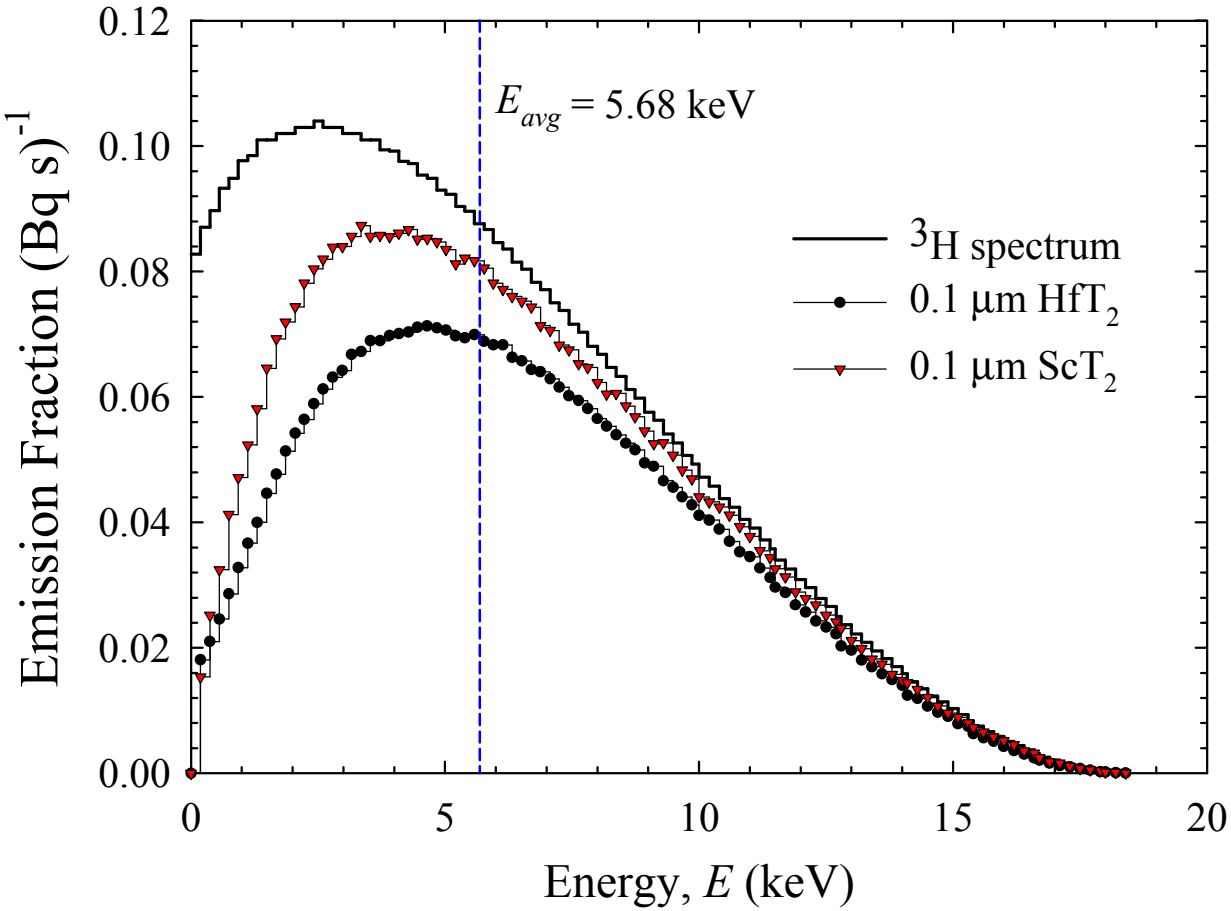
(a) spherical sites used to tabulated microdosimetric quantities (b) annular region used to tally the absorbed dose.

# Electron Emission Spectra (Sc)



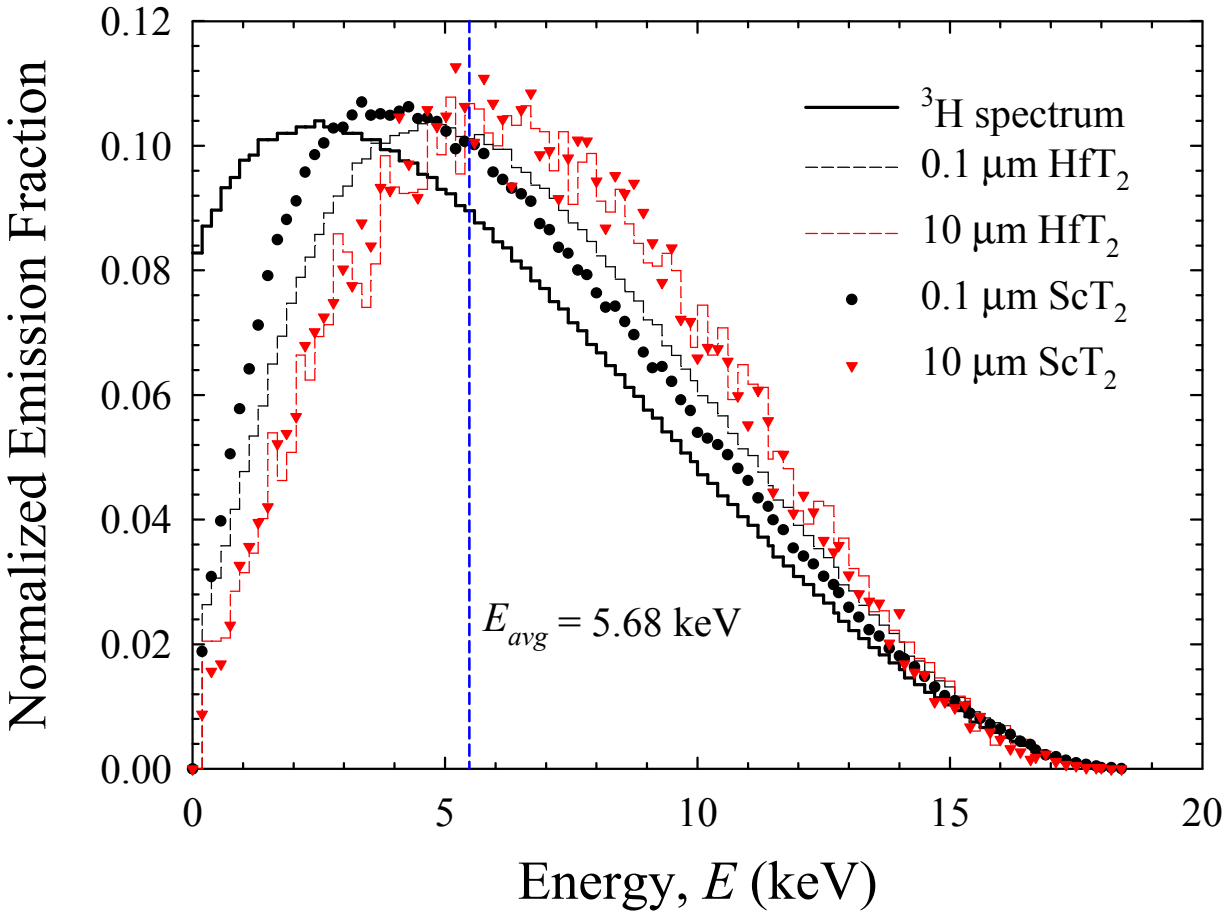

- The larger the particle, the smaller the fraction of radiation that escapes

# Electron Emission Spectra (Sc and Hf)



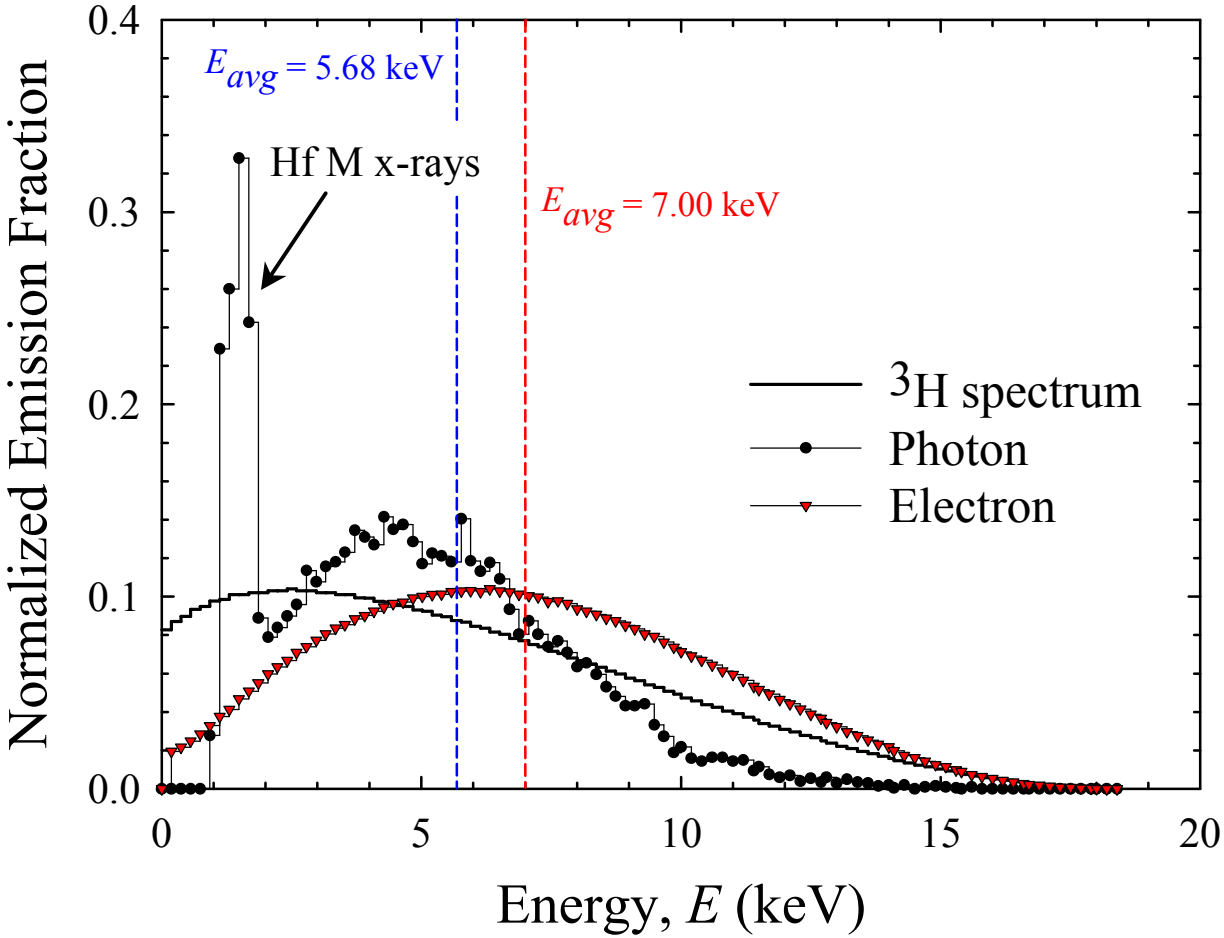

- The fraction of the radiation that escapes
  - decreases with increasing density
  - decreases with increasing atomic number

# Normalized Electron Emission Spectra



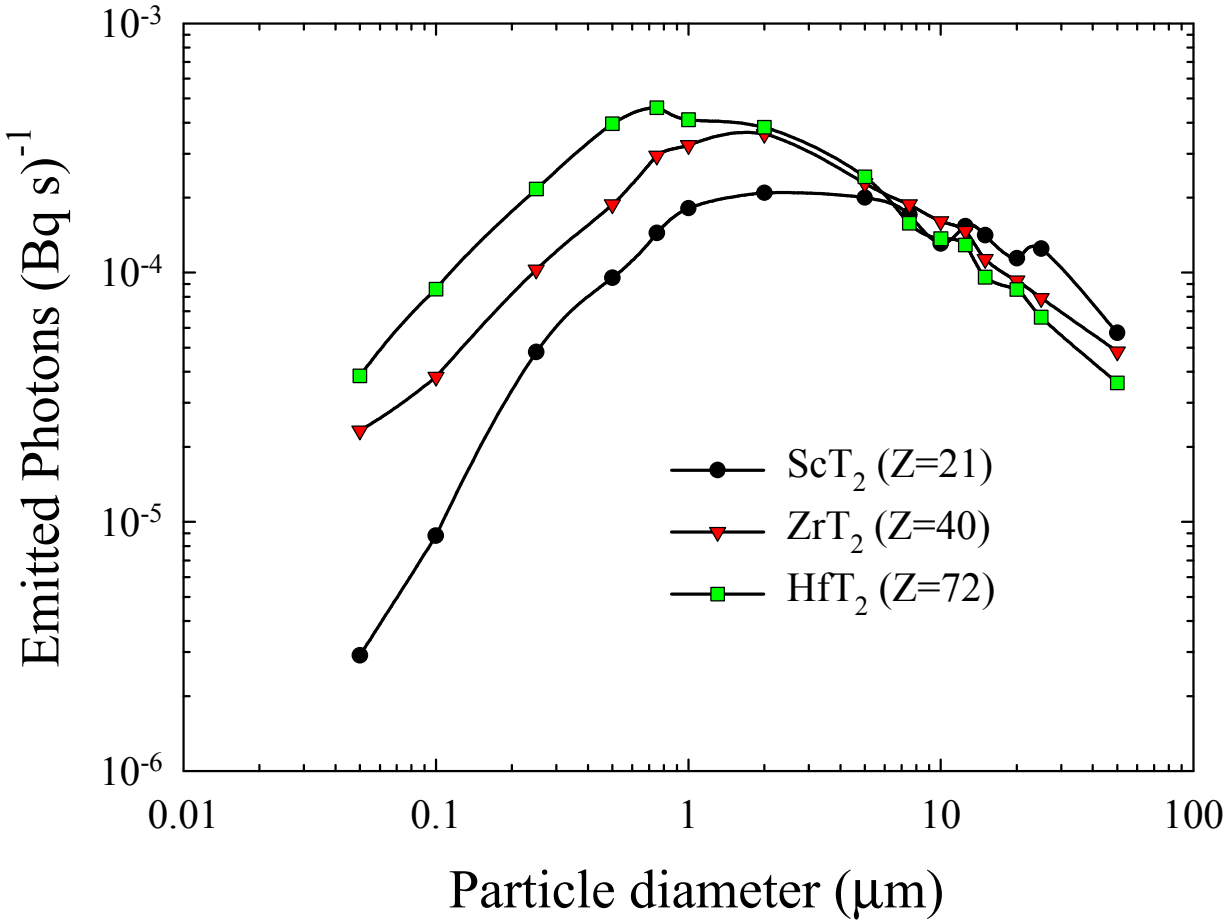

- The emitted electron spectrum tends to "harden" as the particle size increases

# Electron and Photon Emission Spectra




- 5 μm $HfT_2$ particle

# Photons Emitted from Tritide Surface

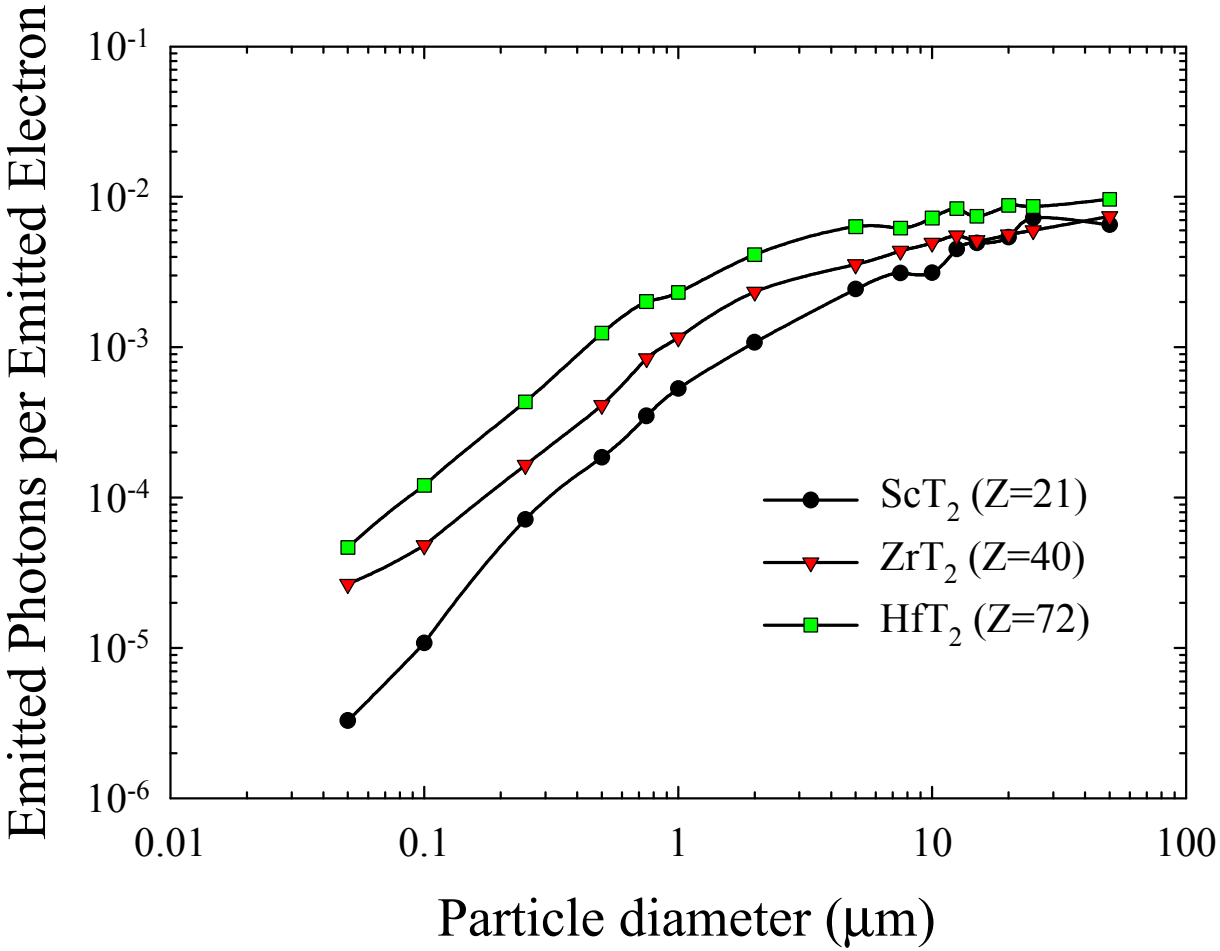



Bremsstrahlung increases

- linearly with particle size below 1 μm
- atomic number for particle sizes below 1 μm

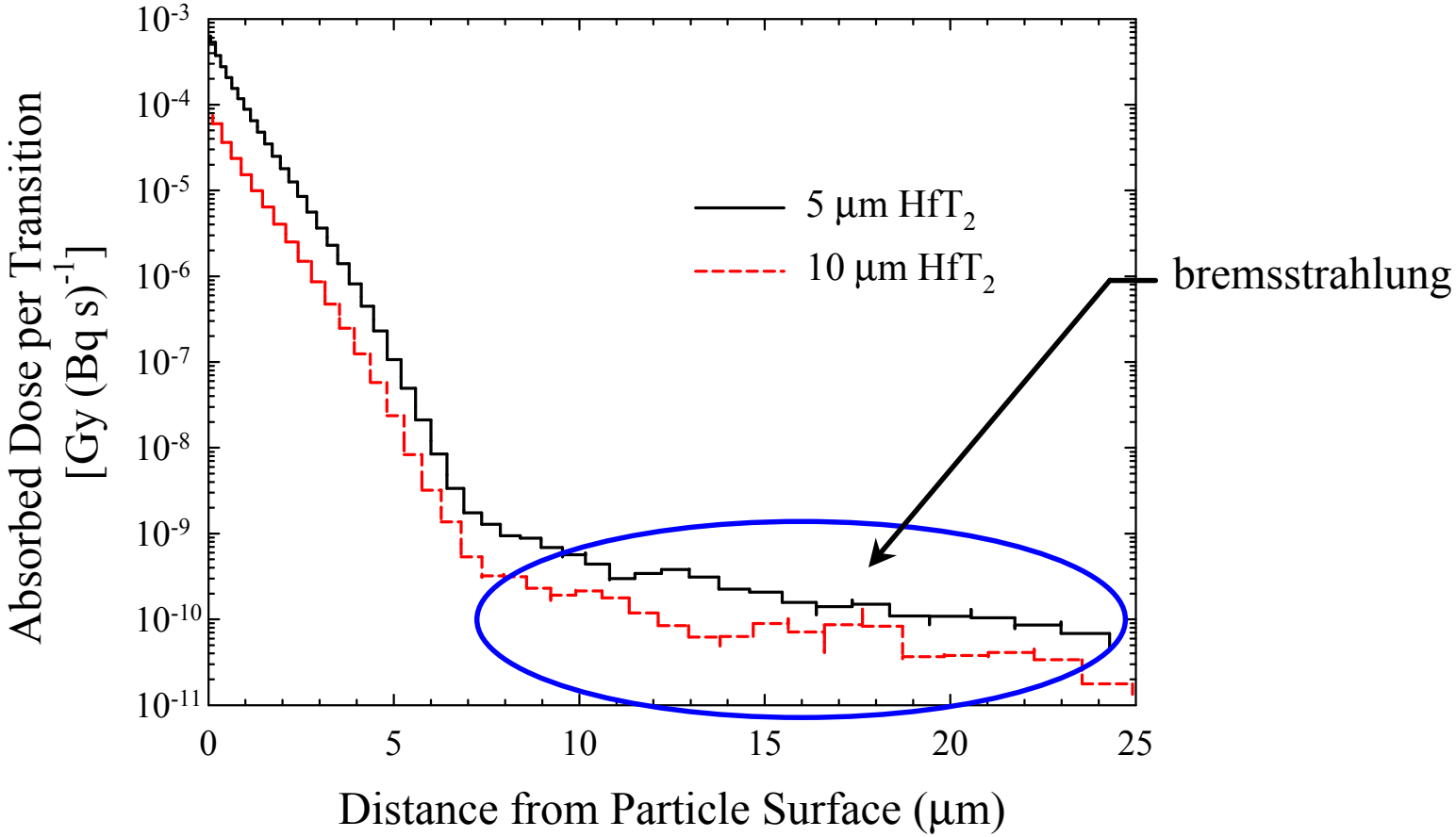
In larger particles, self-absorption overtakes bremsstrahlung production, and drops linearly with particle size

# Photons Emitted from Tritide Surface



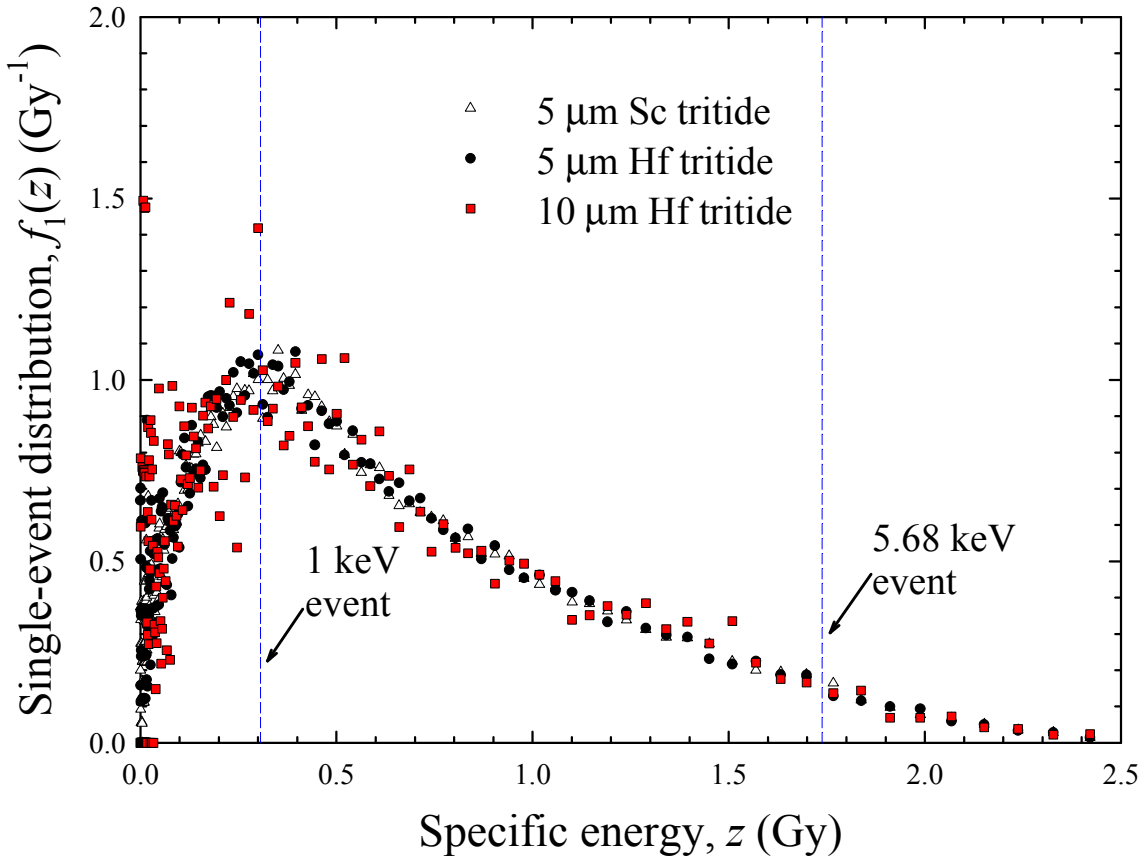

Relative number of emitted bremsstrahlung photons increases as the particle size and atomic number increases

# Radial Dose Distribution (Hf)




- Bremsstrahlung contributes a small fraction to the dose
- But bremsstrahlung is the only type of radiation that contributes to dose for distances greater than about 7 μm

# Single-Event Distribution (1 um site)



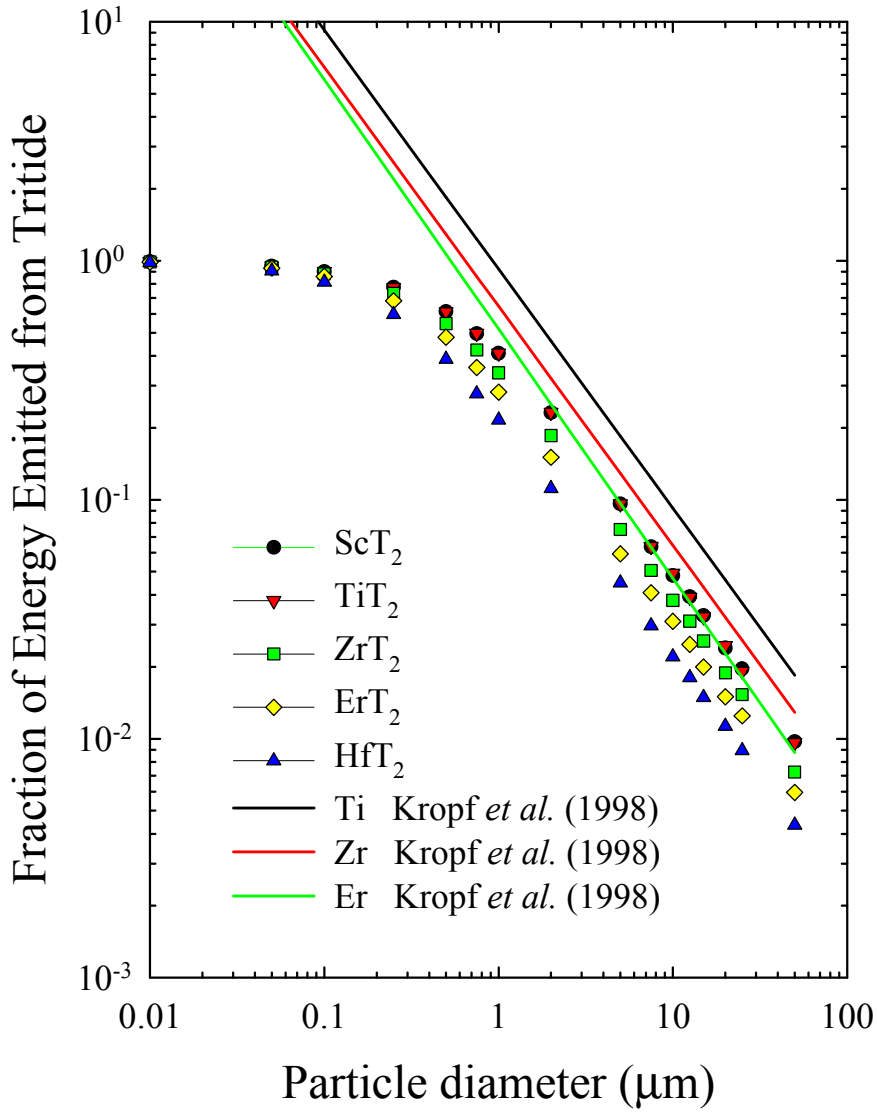

- The energy imparted peaks at an event size of 1 keV

# Hf Tritide Microdosimetry (1 um site)

| Site distance from particle surface (μm) | Energy imparted (keV) | Lineal energy (keV/μm) | Specific energy (mGy) | Probability site "hit" per decay |
|---|---|---|---|---|
| 0.00 | 2.38 | 3.57 | 728.43 | 3.36E-04 |
| 0.50 | 2.41 | 3.62 | 737.69 | 1.34E-04 |
| 1.00 | 2.39 | 3.59 | 732.25 | 5.82E-05 |
| 1.50 | 2.43 | 3.64 | 743.36 | 2.60E-05 |
| 2.00 | 2.55 | 3.83 | 780.46 | 1.15E-05 |
| 2.50 | 2.56 | 3.84 | 782.68 | 5.38E-06 |
| 3.00 | 2.55 | 3.82 | 780.07 | 2.24E-06 |
| 3.50 | 2.60 | 3.90 | 795.59 | 9.47E-07 |
| 4.00 | 2.13 | 3.20 | 651.94 | 2.99E-07 |

Single-event distribution mean energy imparted, lineal energy, and specific energy for a 1 μm site (5 μm Hf tritide particle, $r$ = 11.5 g cm$^{-3}$). Data are based on PENELOPE calculations for $8 \times 10^6$ particle tracks.

# Energy Emitted from Various Tritides



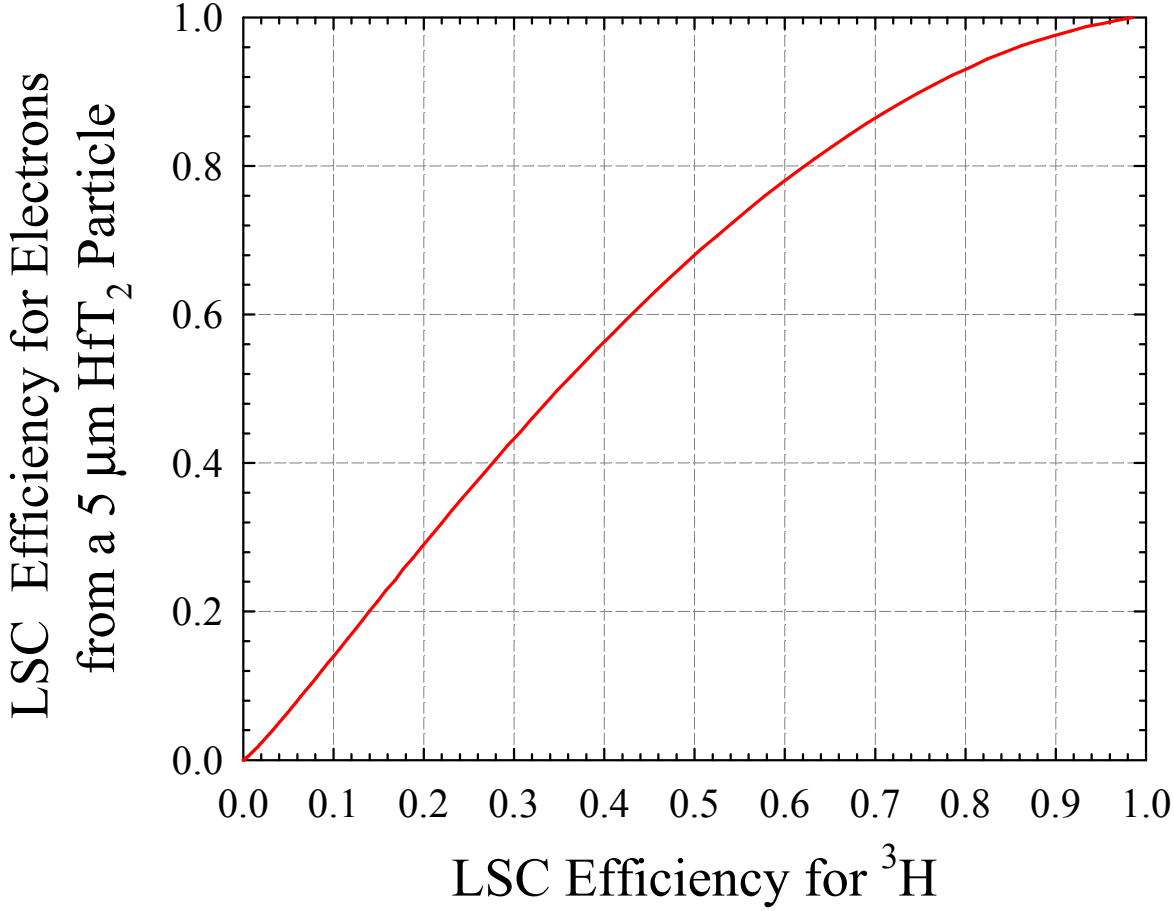

**Kropf *et al.* (1998):**

Energy emission fraction = $bd^{-q}$

| | $b$ | $q$ |
|---|---|---|
| *Ti:* | 0.923 | 1.00 |
| *Zr:* | 0.645 | 1.00 |
| *Er:* | 0.518 | 1.043 |

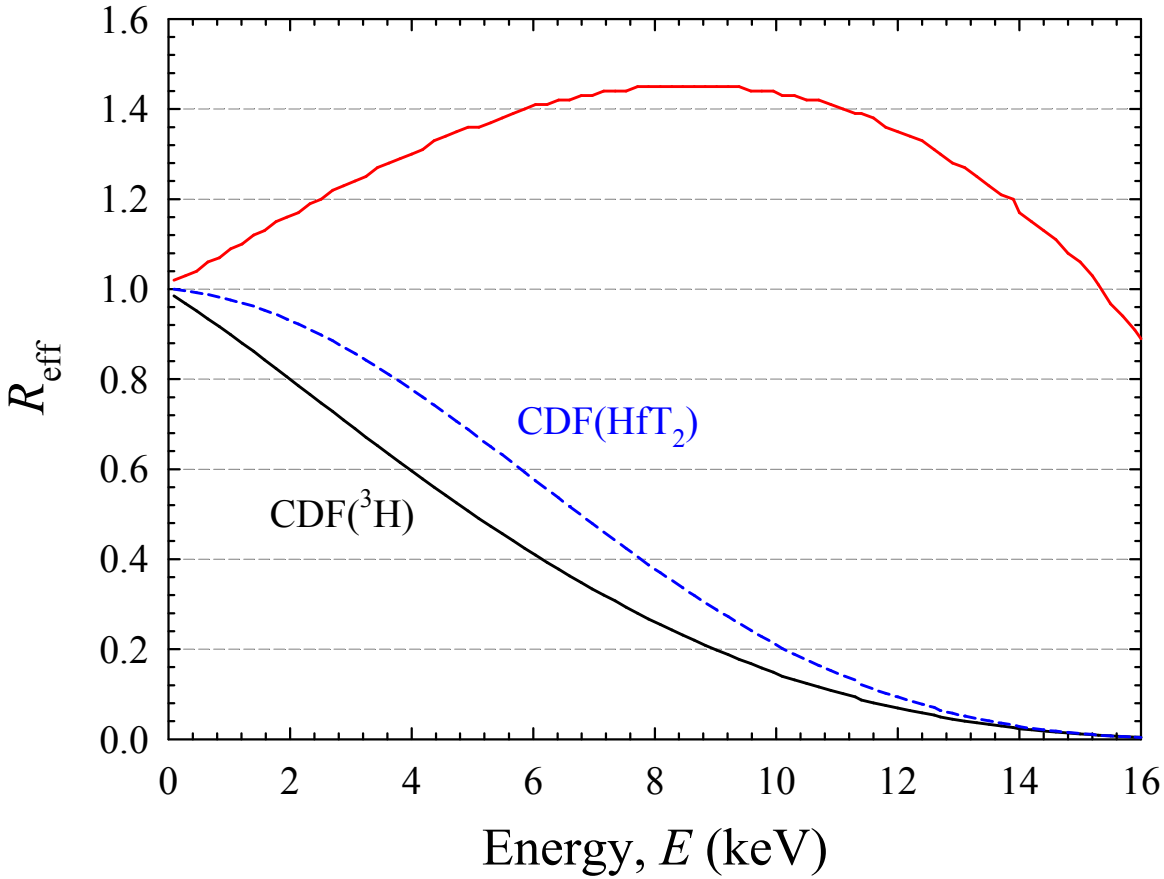
- Over-estimates amount of energy emitted from particle.
- Dose estimates based on Kropf *et al.* formula are too high by at least a factor of 2 or 3.

# Liquid Scintillation Counting Efficiency




Liquid scintillation counting (LSC) efficiency for 5 µm $HfT_2$ versus the LSC for $^3H$. The LSC is calculated based on the assumption that all electrons above a fixed cutoff energy are detected in the scintillation counter.

# Liquid Scintillation Counting Efficiency




$$R_{eff} = \frac{(1 - CDF(HfT_2)}{(1 - CDF(^3H)}$$

- $R_{eff}$ is the ratio of counting efficiency for the tritide particle to the counting efficiency of pure $^3H$
- **"Observed activity" differs from "apparent activity!"**

# Conclusions

- Radiation emitted by Sc, Ti, Zr, Er, and Hf tritides can be considered low-LET radiation
- Uncertainties associated with the composition and density of the tritides are on the order of 20 to 30%
- Electron emission spectrum tends to harden as the particle diameter increases
- Bremsstrahlung production initial increases with particle diameter, reaches a maximum for diameters from about 0.8 and 2.0 μm, and then decreases
  - Impacts calibration of air samplers that measure bremsstrahlung
- The differences between "observed" and "apparent" activity needs to be considered
- Activity median aerodynamic diameter (AMAD) is not appropriate for particles with significant self-absorption

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- Walter E. Wilson, Washington State University

# Supplemental information

**http://www.pnl.gov/eshs/pub/MetalTritide/**