Monte Carlo Solution to Excess Noise and Spatial Blur in Amorphous Selenium Thin-films

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Amorphous selenium (a-Se) is emerging as a viable solid-state imager with avalanche gain for low-light and low-dose radiation detection applications. [1] At high electric fields, hole transport in a-Se can be shifted entirely from localized to extended states, resulting in deterministic and non-Markovian impact ionization avalanche (excees noise factor, $ENF \sim 1$) ~Fig. 1. To understand this behavior, a comprehensive study of the history dependent and non-Markovian nature of the hot hole transport in a-Se was performed using a Monte Carlo (MC) random walk of single hole free flights, interrupted by instantaneous phonon, disorder, hole-dipole, and impact-ionization scattering processes.

Our multi-scale simulation approach combines molecular dynamics (MD) simulations with density functional theory (DFT) and MC simulations (using a non-parabolic band model). The energy and phonon band structure ~Fig. 2, along with the valence band density of states (VB-DOS), for trigonal selenium (t-Se), was calculated using density functional theory (DFT). Fig. 3 shows the DFT calculated acoustic (first order) and optical (zeroth order) deformation potentials along the perpendicular and parallel directions to the c-axis in t-Se. According to our knowledge, this work for the first time uses comprehensive quantum mechanical formulation to calculate energy depended phonon scattering (acoustic, polar emission/absorption and non-polar emission/absorption), hole-dipole disorder scattering (caused by valence alternate pair type defects as scattering centers), and impact ionization scattering rates in a-Se.[2], [3]

Fig. 4 shows the simulated ENF in 0.1-15 μm a-Se thin-films. The non-Markovian nature of hot hole branching dominates for thinner thin films where the dead space distance (min distance traveled to attain impact ionization) is a multiple of the device length. In ~Fig. 5 (a) and (b) we simulated the threshold distance and gain distributions. The history dependent nature of branching of *Hot* holes is explained using a Gaussian distribution of the avalanche threshold distribution distance which increases determinism in the stochastic impact ionization process. An almost ideal non-Markovian hole ENF of ~ 1 was observed in the case of 100 nm a-Se thin-films and avalanche gains of 1000. An inherent limitation to spatial resolution is the laterial blur caused due to the hole drifting process in a-Se, and, we calculate and predict the spatial blur and the full width at half max (FWHM) spread of the avalanching charge cloud in 0.5-200 μm a-Se films ~Fig. 6. Future detector designs can utilize the non-local/non-Markovian nature of hole avalanche in a-Se, to enable a true solid-state photomultiplier with noiseless gain and enhanced signal to noise ratios.

The author D.V. acknowledges the financial support from the National Science Foundation (ECCS 2025490 and ECCS 2048400).

References

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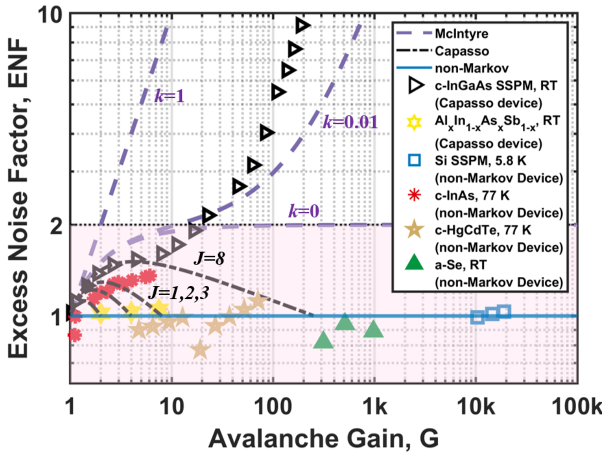

Fig. 1. Excess noise factor in a-Se compared with Markov, non-Markov and Capasso type devices.

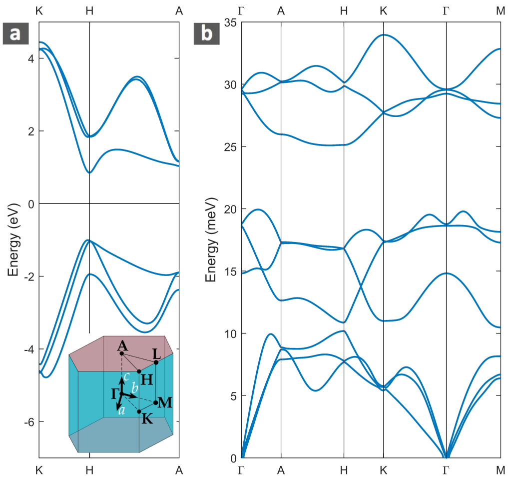

Fig. 2. **(a)** DFT calculated electronic bandstructure for t-Se showing a direct bandgap of 1.9 eV at the H point and **(b)** phonon dispersion. Inset shows the brilloiun zone for t-Se.

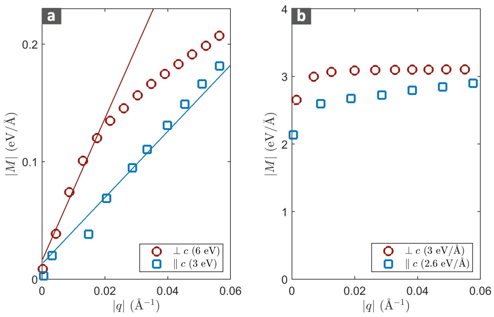

Fig. 3. **(a)** Acoustic (first order) deformation potentials represented by the slope of solid lines and **(b)** optical (zeroth order) deformation potential measured via DFT calculations of hole-phonon coupling using a 225-atom supercell of t-Se along directions perpendicular and parallel to the c-axis.

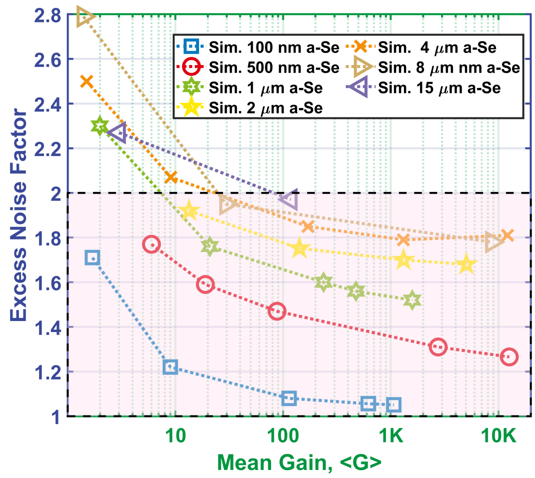

Fig. 4. Plot of ENF from single hole MC simulations for 0.1-15 μm a-Se bulk drift length as a function of mean gain.

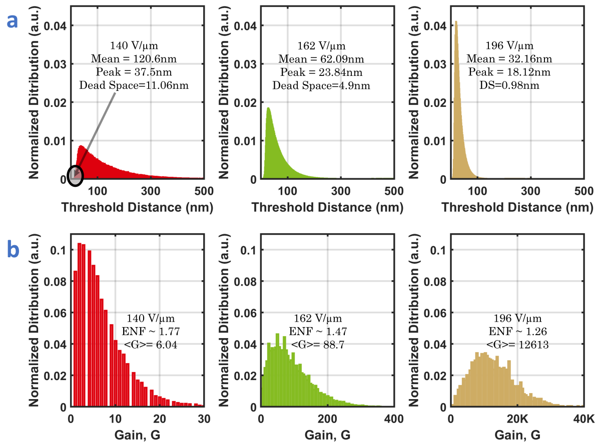

Fig. 5. **(a)** Threshold distance distributions and **(b)** avalanche gain distribution for 500 nm a-Se bulk drift lengths for electric field strengths of 140, 162 and 196 V/μm, respectively.

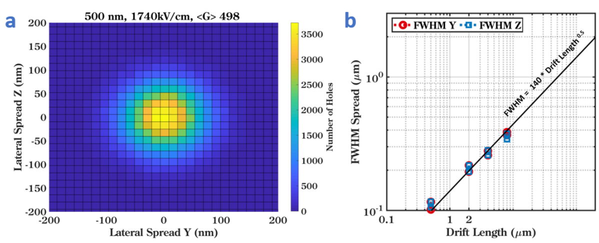

Fig. 6. **(a)** Increase in the spatial spread of a charge cloud of 500 holes injected at $x = 0$. The lateral spread as a function of electric field at the end of 500 nm of travel in a-Se is simulated for 174 V/μm. **(b)** The FWHM simulated for a-Se drift lengths of 500 nm, 2μm, 4μm and 8 μm.