Multiscale Modeling of Hole Avalanche Multiplication and Excess Noise in Amorphous Selenium Semiconductors

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Amorphous selenium (*a*-Se) is a large-area imaging detector material with avalanche gain for low-light and low-dose radiation detection applications.[1] A stark similarity in short range order exists between allotropic forms of selenium, which when augmented with a shift to non-activated extended states transport at high electric fields, allows us to describe the general details of the extended-state hole-phonon interaction in the amorphous phase by modeling band-transport lattice theory of its crystalline counterpart trigonal selenium (*t*-Se). [2] An in-house bulk Monte Carlo algorithm is employed to solve the semiclassical Boltzmann transport equation (MC-BTE). The extended state hole-phonon interaction and the lack of long-range order in *a*-Se is modeled as individual scattering processes, namely acoustic, polar, and non-polar optical phonons, hole-dipole scattering, and impact ionization gain which is modeled using a Keldysh fit. The energy and phonon band structure (**ref. Fig. 1**), along with the valence band density of states (VB-DOS), for *t*-Se, was calculated using density functional theory (DFT) and a non-parabolic approximation to the VB-DOS was used in the simulation (**ref. Fig. 2**). For the first time, we have formulated the interaction of holes in extended states with dipole type defects (the so-called valence alternation pair) present in the chalcogenide family using a non-parabolic VB-DOS approximation. To validate, we compare our drift (**ref. Fig. 3**) and time-of-flight mobility (**ref. Fig. 4**), impact ionization gain (**ref. Fig. 5**), and ensemble energy with experimental findings.[3][4][5][6] This multi-scale approach of combining DFT and MC-BTE is next used in calculating the excess noise factor (ENF) (**ref. Fig. 6**) and spatial resolution in avalanche *a*-Se layers.

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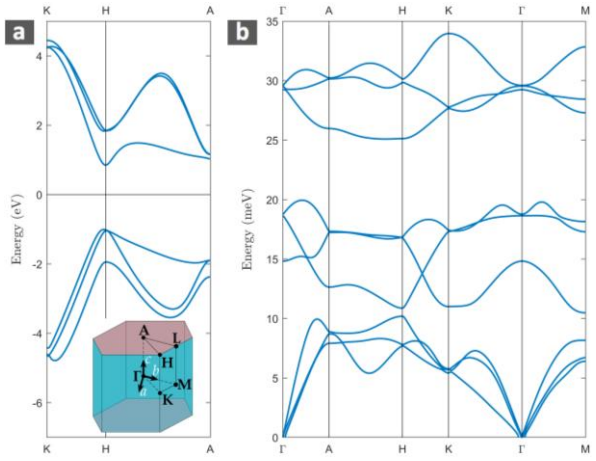

Fig.1: a) DFT calculated electronic band structure for t-Se showing a direct bandgap of 1.9 eV at the H point and (b) phonon dispersion. The brilloiun zone for t-Se is shown as an inset to Fig. 1.

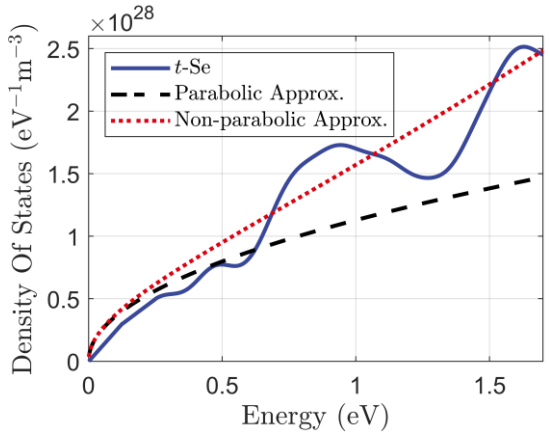

Fig.2: DFT calculations of the VB-DOS are shown by the solid blue line. The dotted red line represents the non-parabolic band approximation (α = 0.15) to the VB-DOS. The dashed line represents the parabolic approximation.

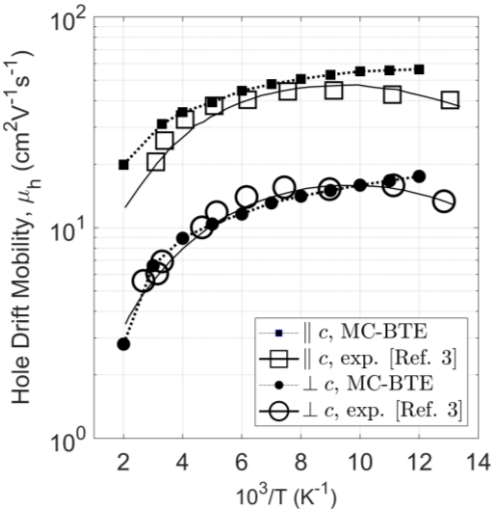

Fig.3: MC-BTE calculated low-field drift mobility values comparison with experiment in the perpendicular and parallel directions to the c-axis in t-Se, respectively. [3]

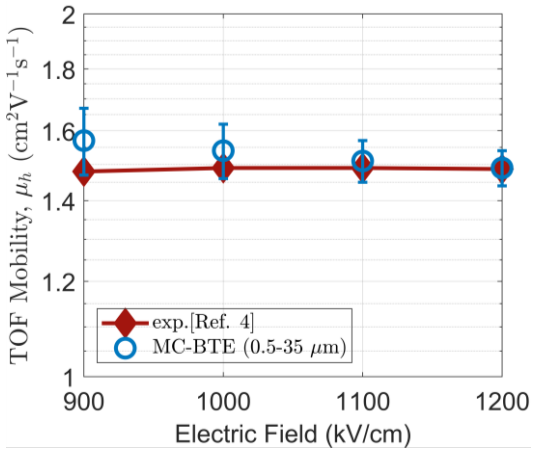

Fig.4: TOF non-parabolic MC-BTE calculated mobility (hollow markers) compared with experimental measured saturated and electric field-independent mobility (solid markers) in a-Se. [4]

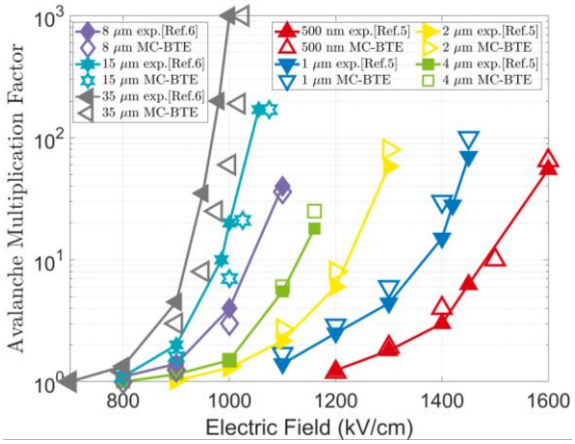

Fig.5: Impact Ionization gain calculated using non-parabolic MC-BTE and compared with experimentally measured gain for 0.5-35 μm thick a-Se films.[5][6]

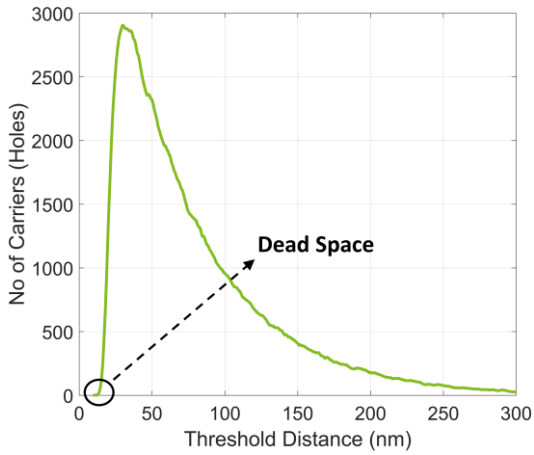

Fig.6: Threshold distance distribution showing the presence of a "dead-space" (defined as the minimum distance of travel in the direction of electric field before a carrier undergoes impact ionization avalanche) in 500 nm a-Se layers, resulting in a calculated ENF of ~1.4.