IIETA International Information and Engineering Technology Association
Advancing the World of Information and Engineering

Mathematical Modelling of Engineering Problems
Vol. 12, No. 12, December, 2025, pp. 4249-4256
Journal homepage: http://iieta.org/journals/mmep

Ensemble Monte Carlo Analysis of Electronic Transport Properties Including Ionization Impact in $Hg_{0.66}Cd_{0.34}Te$ for Thin Film Solar Applications

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https://doi.org/10.18280/mmep.121213

Received: 20 August 2025
Revised: 3 November 2025
Accepted: 12 November 2025
Available online: 31 December 2025

Keywords:
Boltzmann Equation, electronic transport, $Hg_{1-x}Cd_xTe$, Monte Carlo simulation, scatterings, ternary alloy

ABSTRACT

This study investigates the potential of using $Hg_{0.66}Cd_{0.34}Te$ for high-efficiency photovoltaic applications by analyzing its high-field electron transport properties. The problem of performance limitations in conventional solar cells has motivated the search for materials exhibiting carrier multiplication and velocity overshoot. Using an ensemble Monte Carlo (EMC) methodology, we simulate electron dynamics to solve the Boltzmann transport Equation within a three-valley band structure. Our key findings reveal a significant room-temperature velocity overshoot phenomenon and identify a critical doping range where impact ionization becomes the dominant generation mechanism. Furthermore, the material demonstrates exceptional operational temperature stability. These results imply that $Hg_{0.66}Cd_{0.34}Te$ is a highly promising absorber material for next-generation, ultra-high-efficiency photovoltaic devices, such as carrier multiplication and tandem solar cells.

1. INTRODUCTION

The ternary alloy $Hg_{1-x}Cd_xTe$ is a semiconductor of paramount importance for infrared optoelectronics and emerging photovoltaic technologies. Its electrical and optical properties are governed by the energy band structure inherited from CdTe and HgTe [1], particularly near the Γ-point of the Brillouin zone. A key feature of $Hg_{1-x}Cd_xTe$ is its tunable direct band-gap, which depends directly on the CdTe mole fraction (x) and temperature [2], allowing it to cover the entire infrared spectrum. Furthermore, it boasts a high absorption coefficient, exceptional electron mobility, and a prolonged carrier lifetime, making it one of the best material for infrared photodetectors [3] and a promising candidate for high-efficiency, thin-film solar cells [4].

Despite its well-established low-field properties, a significant challenge remains in accurately modeling and understanding its high-field electron transport behavior. Phenomena such as intervalley scattering, velocity overshoot, and impact ionization in the complex three valley (Γ, L, X) band structure of Mercury Cadmium Tellurid (MCT) are not fully characterized, especially under conditions relevant to advanced photovoltaic operation. Existing models often lack the granularity to predict the interplay between doping, field strength, and carrier multiplication efficiency, which is critical for designing devices that surpass the Shockley-Queisser limit.

The primary objective of this work is to resolve these challenges by employing a detailed ensemble Monte Carlo simulation. This study aims to:

- Model high-field transport in $Hg_{0.66}Cd_{0.34}Te$, incorporating a full three-valley band structure and key scattering mechanisms, including impact ionization.
- Quantify transient effects, such as velocity overshoot, and steady-state properties like the impact ionization coefficient.
- Identify the optimal doping concentrations that enhance carrier multiplication by favoring impact ionization over Auger recombination.

All simulations in this study were performed with the applied electric field in the "111" crystallographic direction. This orientation is chosen for its practical relevance, as it ensures perfect symmetry across all equivalent valleys, meaning carriers are heated identically by the field regardless of their initial valley. Consequently, the distribution function, average velocity, and energy are identical for all valleys under this symmetric condition, simplifying the analysis without loss of generality for the transport properties investigated.

2. MODEL DESCRIPTION

This study employs an ensemble semi-classical Monte Carlo method to simulate electron transport in $Hg_{1-x}Cd_xTe$. The core of this approach is the stochastic solution of the

Boltzmann Transport Equation (BTE) by tracking a large number of electron trajectories in phase space (real space and wave-vector space) over time [5, 6]. The key advantage of this method is the explicit inclusion of major scattering mechanisms without relying on a temporal relaxation approximation, which is crucial for accurately modeling high-field phenomena like velocity overshoot and impact ionization.

The model is built upon semi-classical principles: electrons are treated as classical particles that propagate ballistically under the influence of an external electric field according to Newton's laws, while scattering events (e.g., with phonons or impurities) are treated quantum-mechanically using Fermi's Golden Rule and scattering rates. A fundamental limitation of this approach is the neglect of full quantum coherence and tunneling effects; however, it remains the most accurate method for simulating high-field, non-equilibrium transport in bulk semiconductors and microstructures where phase coherence is not the dominant effect.

Table 1. Material parameters for $Hg_{0.66}Cd_{0.34}Te$ at 300 K and 77 K

Parameter	Symbol	T = 300 K	T = 77 K	Units
Bandgap	E_9	-0.083	-0.149	eV
Γ-L Valley Separation	ΔE_{9l}	1.76	1.79	eV
Γ-X Valley Separation	ΔE_{9x}	2.16	2.19	eV
Electron Effective Mass	m_e^*/m_0	0.032	0.031	-
Lattice Constant	a_0	6.468	6.468	Å
Mass Density	ρ	7,430	7,430	kg/m³
Sound Velocity	S	2,770	2,770	m/s
Static Permittivity	ε_s	16.1	16.8	-
High-frequency Permittivity	$\varepsilon\infty$	13.8	14.0	-
Optical Phonon Energy	$\hbar\omega_0$	15.4	15.6	meV
Acoustic Deformation Potential	U_ac	10.0	10.0	eV
Alloy Scattering Potential	U_{all}	1.5	1.5	eV
Characteristic Thermal Energy	k_pT	25.85	6.63	meV

The electronic structure is the most critical input for the simulation [7]. Our model employs a three-valley conduction band (Γ, L, and X), where each valley is treated as isotropic but non-parabolic. The model integrates the deformation potential of each valley, the energy band gap structures, and the key scattering mechanisms. The relative electron concentrations in the L and X valleys are calculated based on their effective densities of state and energy separations from the Γ-valley minimum [8]:

$$N_\Gamma = 2\left(\frac{2\pi m_e^\Gamma KT}{\bar{h}^2}\right)^{3/2} exp\left(E_p/KT\right) \quad (1)$$

$$\frac{N_L}{N_\Gamma} = \left(\frac{m_e^L}{m_e^\Gamma}\right)^{3/2} exp - \left(\frac{\Delta E_{\Gamma L}}{KT}\right) \quad (2)$$

$$\frac{N_X}{N_\Gamma} = \left(\frac{m_e^X}{m_e^\Gamma}\right)^{3/2} exp - \left(\frac{\Delta E_{\Gamma X}}{KT}\right) \quad (3)$$

where, $E_{\Gamma L}$ and $E_{\Gamma X}$ are the separation energies between *Γ-L* and *Γ-X* valleys respectively.

Alongside the electronic structure, carrier-phonon interactions at high energies are essential for accurately modeling carrier dynamics under high electric fields [9].

2.1 Scattering mechanism rates

The model incorporates the dominant scattering mechanisms in HgCdTe: acoustic deformation potential scattering, polar optical -phonon scattering, and alloy disorder scattering. All scattering rates are calculated using Fermi's golden rule, derived from first-order time-dependent perturbation theory.

The following subsections detail the formulation for each mechanism. The material properties and constants used in these calculations are summarized in Table 1.

2.1.1 Acoustic deformation scattering

Acoustic phonon scattering is a quasi-elastic process described by deformation potential theory, where the crystal strain perturbs the electronic energy. In HgCdTe, its influence is generally secondary to polar optical and alloy scattering. The scattering rate for an electron with wavevector k (cm^{-1}) and energy δ(E) (eV) is given by [8]:

$$R_a(k) = \frac{(2m_e * m_0)^{3/2} K_B T U_{ac}^2}{2\pi\rho S^2 \hbar^4} \delta^{1/2}(E)(1+\alpha E) F_a(E) \quad (4)$$

$$F_a(E) = \frac{(1+\alpha E)^2 + \frac{1}{3}(\alpha E)^2}{(1+2\alpha E)^2} \quad (5)$$

2.1.2 Polar optical scattering (emission and absorption)

At room temperature and low electric fields, polar optical-phonon scattering dominates within the Γ-valley. This inelastic mechanism changes the carrier energy by the phonon energy $\hbar\omega_0$ and is highly anisotropic.

HgCdTe exhibits "two-mode" behavior, meaning optical phonon modes from both parent compounds (HgTe and CdTe) persist. Therefore, the effective phonon energy is composition-weighted:

$$\hbar\omega_0 = (1-x)\hbar\omega_{HgTe} + x\hbar\omega_{CdTe} \quad (6)$$

The total polar optical scattering rate, accounting for both absorption and emission processes, is given by [10]:

$$R_{po}(k) = \frac{q^2\sqrt{m_e * m_0}\hbar\omega_0}{4\pi\sqrt{2}\hbar\varepsilon_0}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_S}\right)\frac{1+2\alpha E'}{\delta^{1/2}(E)} F_0(E,E') \quad (7)$$

The final energy E' after a scattering event is:

$$E' = \begin{pmatrix} E + \hbar\omega_0 \; For\; absorption \\ E - \hbar\omega_0 \; For\; emission \end{pmatrix} \quad (8)$$

The function $F_0(E,E')$ and its components are defined as:

$$F_0(E,E') = C^{-1}\left[A \ln\frac{\delta^{1/2}(E) + \delta^{1/2}(E')}{\delta^{1/2}(E) - \delta^{1/2}(E')} + B\right] \quad (9)$$

$$A = [2(1+\alpha E)(1+\alpha E') + \alpha\{\delta(E) + \delta(E')\}]^2 \quad (10)$$

$$B = 2\alpha\delta^{1/2}(E)\delta^{1/2}(E') \\ [4(1+\alpha E)(1+\alpha E') + \alpha\{\delta(E)+\delta(E')\}] \quad (11)$$

$$C = 4(1+\alpha E)(1+\alpha E')(1+2\alpha E)(1+2\alpha E') \quad (12)$$

The phonon occupation number $n(\omega_0)$ follows the Bose-Einstein distribution:

$$n(\omega_0) = \frac{1}{exp\left(\frac{\hbar\omega_0}{K_B T}\right)} \quad (13)$$

2.1.3 Alloy scattering

In ternary alloys like $Hg_{1-x}Cd_xTe$ intrinsic disorder causes carrier scattering due to random fluctuations of the crystal potential at the unit cell level. The scattering rate for a perfectly random alloy is given by [11]:

$$R_{all}(k) = 1.5 * 10^{13}(m_e^*)^{3/2}U_{all}{}^2 a_0{}^3 \\ x(1-x)\delta^{1/2}(E)(1+2\alpha E) \quad (14)$$

where, $V_0 = a_0{}^3/4_0$ is the volume of the unit cell [12].

2.2 Monte Carlo simulation algorithm

This study employs an ensemble Monte Carlo method to simulate electron transport in the ternary alloy $Hg_{0.66}Cd_{0.34}Te$. The simulation tracks an ensemble of 30,000 electrons over a duration of 4 ps, a configuration chosen to ensure statistical significance while maintaining computational tractability.

The core of our simulation follows the standard ensemble approach but is distinguished by its incorporation of a three-valley model (Γ, L, X) for HgCdTe and specific scattering mechanisms critical for this material, including impact ionization. Rather than delving into extensive mathematical derivations, this section outlines the unique aspects of our implementation. A high-level pseudocode summary is provided in Algorithm 1 to illustrate the overall workflow.

- Electrons are permitted to scatter between the Γ, L, and X valleys based on energy-dependent transition rates. The effective mass and density of states are uniquely parameterized for each valley in the HgCdTe alloy.
- The model includes the following mechanisms: acoustic phonon deformation potential scattering, polar optical phonon scattering, intervalley scattering (between Γ-L and Γ-X valleys), and impact ionization. The rates for these processes were calculated using the non-parabolic band approximation.
- All electrons are initialized in the lowest-energy Γ-valley with wave vectors drawn from a Maxwell-Boltzmann distribution corresponding to the lattice temperature (T), ensuring a state of thermal equilibrium.

The free flight duration is determined using a constant, self-scattering-corrected total rate Γ to simplify the computation of the stochastic flight time [13]. After each free flight, a scattering mechanism is selected by comparing a second random number to the normalized cumulative scattering probabilities. The final state (wave vector and valley) after scattering is determined stochastically based on the specific selected mechanism [14].

Impact ionization events are treated as a special scattering process that generates new electron-hole pairs, which are subsequently included in the ensemble.

Algorithm 1. Ensemble Monte Carlo Simulation for $Hg_{0.66}Cd_{0.34}Te$

1. INITIALIZATION
   - Set material parameters (alloy composition, band structure for Γ, L, X valleys).
   - Set simulation controls (N_electrons = 30,000, total_time = 4 ps, time_step Δt).
   - Set external conditions (electric field E, lattice temperature T).
   - Precompute and tabulate scattering rates R_i(ε) for all mechanisms as a function of electron energy.
2. INITIALIZE ELECTRONS
   for each electron in ensemble do
      valley_id = Γ
      k = random wave vector from thermal distribution
      r = 0 (initial position)
      energy = calculate from k and valley band structure
   end for
3. MAIN LOOP: PROPAGATE IN TIME
   while simulation_time < total_time do
      for each electron in ensemble do
         // A. DETERMINE FREE FLIGHT DURATION
         Generate random number r1 ~ U(0,1).
         total_scattering_rate = sum of all R_i(current_energy) + self_scattering_rate
         free_flight_time τ = -ln(r1) / total_scattering_rate
         // B. DRIFT ELECTRON
         Propagate electron ballistically under electric field E for time τ.
         Update k(t) and r(t) according to Newton's laws (using valley-specific effective mass).
         Update electron energy ε.
         // C. SELECT SCATTERING MECHANISM
         Generate random number r2 ~ U(0,1).
         Find mechanism n such that: S_{n-1} < r2 * total_scattering_rate ≤ S_n
         (where S_n is the cumulative sum of scattering rates up to mechanism n).
         // D. APPLY SCATTERING
         if selected_mechanism is not self-scattering then
            // Valley Selection occurs here
            if mechanism is intervalley or ionization then
               Select new target valley based on scattering tables.
            end if
            // Update final state
            k_final = stochastically determined from the selected scattering mechanism.
            valley_id = new_valley (if valley-changing scattering occurred).
         end if
         // If self-scattering, k and valley remain unchanged.
      end for
      // E. ENSEMBLE DATA COLLECTION
      Calculate average drift velocity and energy for electrons in each valley (Γ, L, X).
      Store results for this time step.
      simulation_time = simulation_time + Δt
   end while
4. OUTPUT AND ANALYSIS
   - Compute time-averaged transport properties (e.g., steady-state velocity, average energy).

The simulation outputs the time-dependent ensemble averages for the drift velocity and energy, calculated separately for each valley using the following expressions [15, 16]:

$$v_d = \frac{1}{N}\sum_{i=1}^{N} v_i(t) \tag{15}$$

$$\varepsilon = \frac{1}{N}\sum_{i=1}^{N} \varepsilon_i(t) \tag{16}$$

$$v_i(t) = \frac{\hbar . k_{xi}}{m^*(1 + 2\alpha\varepsilon_i)} \tag{17}$$

$$\varepsilon_i(t) = \frac{-1 + \sqrt{1 + 4\alpha\, y}}{2\alpha} \tag{18}$$

where, $v_i(t)$ is the velocity of an individual electron and its energy is given by $\varepsilon_i(t)$.

As highlighted in several theoretical and experimental studies, impact ionization is a significant scattering process in semiconductors, where a high-energy particle generates an electron–hole pair (e.g., as observed in solar cells). This process plays a critical role in device reliability, such as in MOSFETs, where the substrate current acts as an indicator of hot electrons responsible for oxide degradation or avalanche breakdown, potentially leading to device failure [17].

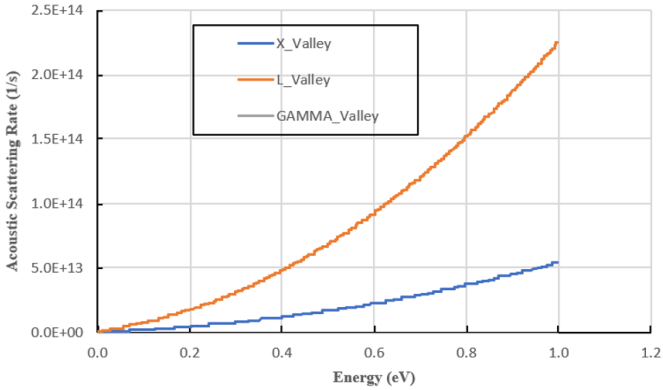
Impact ionization is included as an additional interaction mechanism in the calculation of electron transport parameters, complementing acoustic scattering, polar absorption, polar emission, and alloy scattering [18]. The impact ionization coefficient for electrons (α) is defined as the number of electron–hole pairs generated by a single electron as it travels 1 cm through the depletion layer in the direction of the electric field [19-21].

3. RESULTS AND DISCUSSIONS

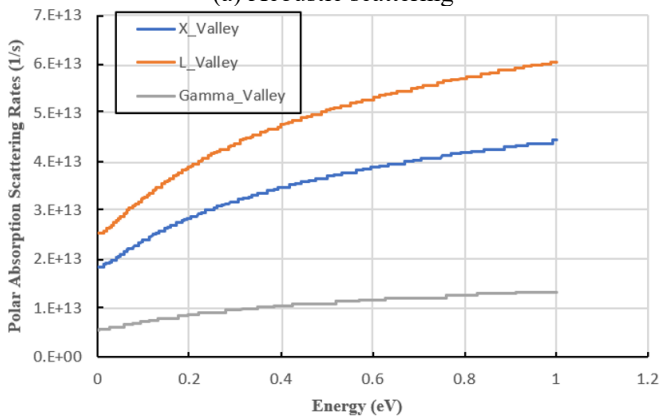
This section presents the key findings from our ensemble Monte Carlo simulation of electron transport in $Hg_{0.66}Cd_{0.34}Te$. We analyze steady-state and transient characteristics, with a particular focus on valley transfer, velocity overshoot, and impact ionization. The results are consolidated for clarity, supported by statistical analysis, and discussed in the context of experimental literature and their implications for photovoltaic device performance.

3.1 Steady-state transport and scattering analysis

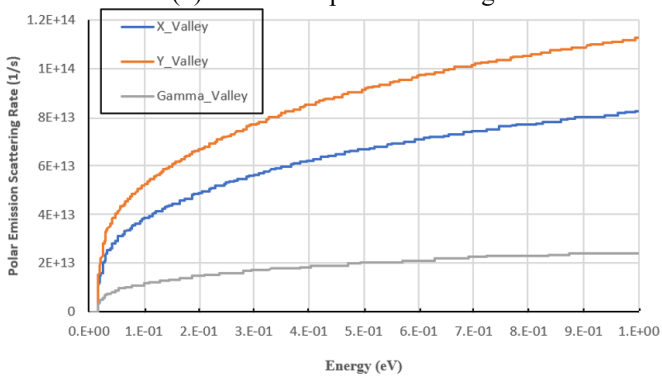
The electron dynamics in HgCdTe are governed by several scattering mechanisms, whose energy-dependent rates are plotted in Figure 1. Acoustic scattering, as shown in Figure 1(a), shows a linear increase with energy, becoming significant in the high-effective-mass X-valley. Polar optical phonon scattering in Figures 1(b) and (c) is a dominant inelastic mechanism across all valleys, with the emission rate surpassing absorption and rising sharply with energy. Alloy scattering presented in Figure 1(d), arising from compositional fluctuations [22], becomes a dominant channel at high energies and fields.



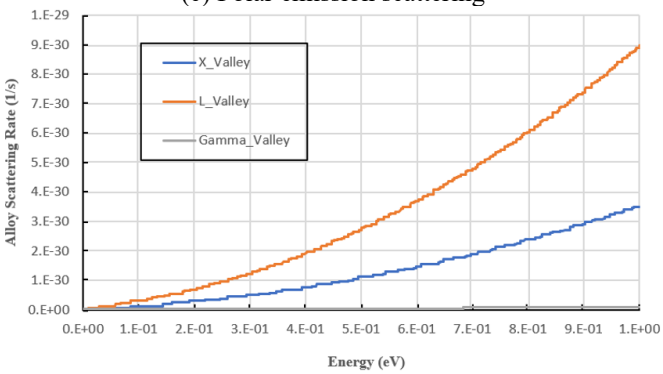
(a) Acoustic scattering



(b) Polar absorption scattering



(c) Polar emission scattering



(d) Alloy scattering

Figure 1. Calculated scattering probabilities versus carrier energy for: (a) acoustic phonon, (b) polar optical phonon absorption, (c) polar optical phonon emission, and (d) alloy disorder interactions

The interplay of these rates dictates valley population. As shown in Figure 2, electrons begin transferring from the central Γ-valley to the L-valley at ~0.5 kV/cm. The L-valley population surpasses that of the Γ-valley shortly after this

threshold. Transfer to the X-valley initiates around 9 kV/cm, but its population remains insignificant even at high fields.

The interplay between carrier acceleration and these scattering mechanisms determines the macroscopic transport properties. Figure 3 shows the average electron drift velocity as a function of the applied electric field. The velocity initially increases, peaking at a saturation value of $(7.53 \pm 0.28) \times 10^7$ cm/s (95% confidence interval from ensemble statistics) at a critical field of ~1 kV/cm. This is followed by a characteristic negative differential mobility regime, where velocity drops sharply to 1.89×10^7 cm/s at 6.3 kV/cm due to increased intervalley scattering. At higher fields, the velocity gradually decreases to 7.71×10^6 cm/s at 80 kV/cm.

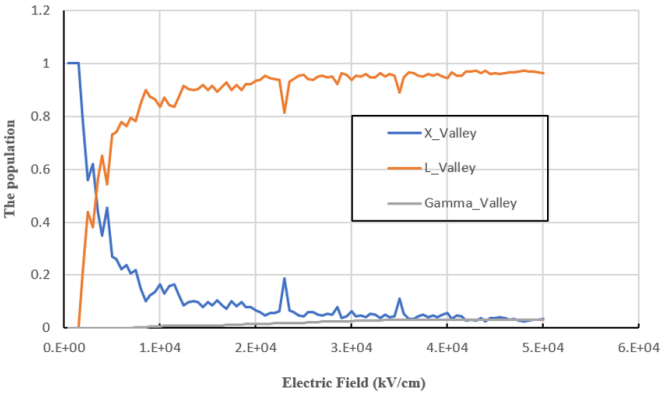


Figure 2. Electric field dependence of valley occupation probabilities for Γ, L, and X conduction bands in HgCdTe at 300 K under steady-state conditions

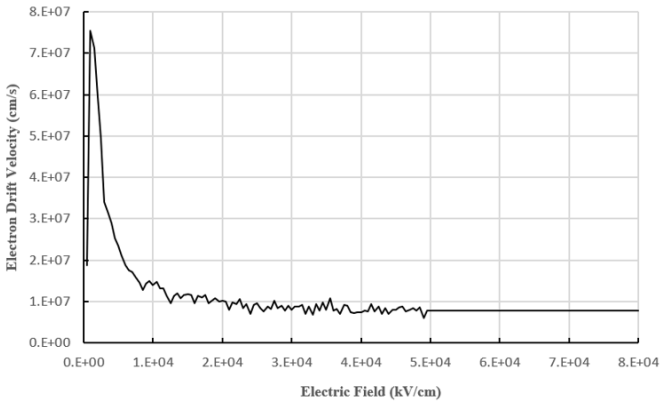


Figure 3. Simulated electron drift velocity characteristics as a function of applied electric field at room temperature

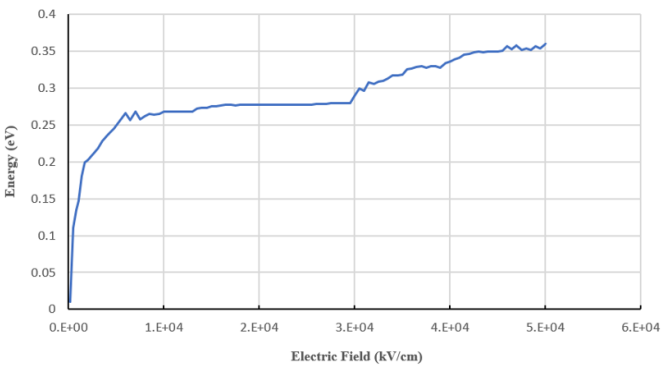


Figure 4. Evolution of average electron energy with increasing electric field strength in $Hg_{0.66}Cd_{0.34}Te$ at 300 K

Table 2. Consolidated summary of key transport properties in $Hg_{0.66}Cd_{0.34}Te$ at 300 K

Parameter	Value	Condition (Electric Field)
Peak drift velocity	$(7.53 \pm 0.28) \times 10^7$ cm/s	~1 kV/cm
Velocity overshoot duration	0.15–0.3 ps	> 5 kV/cm
Stready state velocity	7.71×10^6 cm/s	> 80 kV/cm
Electron energy	0.266 eV	> 1 kV/cm
Critical field for Γ→L transfer	~1.1 kV/cm	-
Impact ionization threshold field	1.2–5.5 kV/cm	-
Optimal doping range	$1e^{20}$ cm^{-3}–$1e^{24}$ cm^{-3}	For ionization dominance

The corresponding electron energy behavior is shown in Figure 4. The energy rises rapidly upon field application, reaching a maximum of 0.266 eV. A secondary peak is observed at ~6.33 kV/cm, coinciding with the steepest part of the velocity drop in Figure 3, highlighting the dynamic energy exchange during valley transfer. Subsequently, the carrier energy stabilizes despite increasing field.

Key results are summarized in Table 2, where applicable statistical confidence intervals, comparisons with experimental and theoretical literature are provided to validate our findings.

3.2 Transient analysis and hot-carrier dynamics

To probe non-stationary effects, we simulated the temporal response to a sudden application of high electric fields. Figures 5 and 6 show the transient average velocity and energy, respectively.

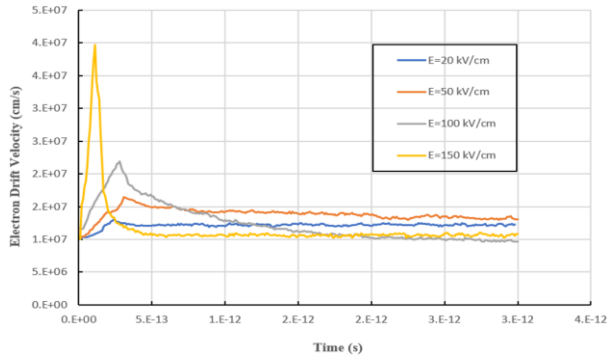


Figure 5. Transient average electron velocity at ambient temperature for different values of the applied electric field

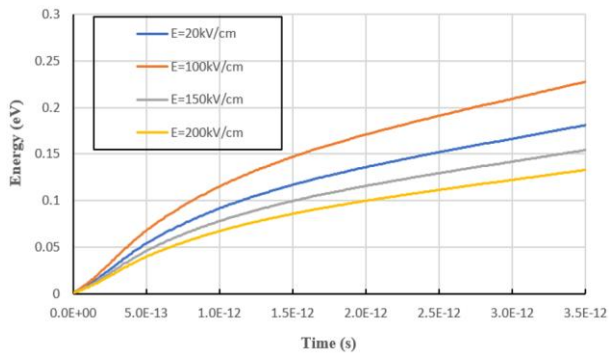


Figure 6. Transient electron energy at ambient temperature for different values of the applied electric field

A pronounced velocity overshoot is observed for fields significantly exceeding the critical field (~1 kV/cm). This overshoot occurs due to a transient regime where electrons are accelerated to high velocities in the low-mass Γ-valley before they gain sufficient energy to scatter into the high-mass L-valley. The duration of this velocity overshoot is quantified to be between 0.15 and 0.3 picoseconds, a timescale consistent with hot-carrier dynamics reported in semiconductors like GaAs and InP [23], though the effect is more pronounced in HgCdTe at room temperature due to its specific band structure.

Our simulation reveals a significant velocity overshoot at 300 K. While some scholars [23-25] predicted this phenomenon in IR-composition HgCdTe at cryogenic temperatures, our work demonstrates its strength at ambient temperature, a critical advance for practical hot-carrier photovoltaic applications. This performance is consistent with reduced dimensionality effects predicted by stochastic transport theory [26] and finds strong validation in recent experimental studies of HgCdTe quantum dots [27-29].

3.3 Doping, impact ionization, and device-level implications

The effect of doping concentration ($1e^{20}$ cm^{-3}–$1e^{24}$ cm^{-3}) on transient transport is shown in Figures 7 and 8. Increased impurity concentration reduces low-field mobility and suppresses the peak overshoot velocity due to enhanced ionized impurity scattering. Our results identify a clear optimal doping window between $1e^{20}$ cm^{-3}–$1e^{24}$ cm^{-3} where impact ionization can dominate over Auger recombination losses.

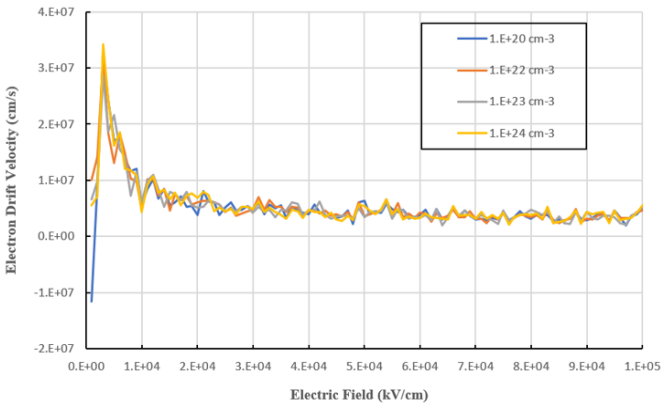


Figure 7. Effect of impurity concentration on transient electron drift velocity

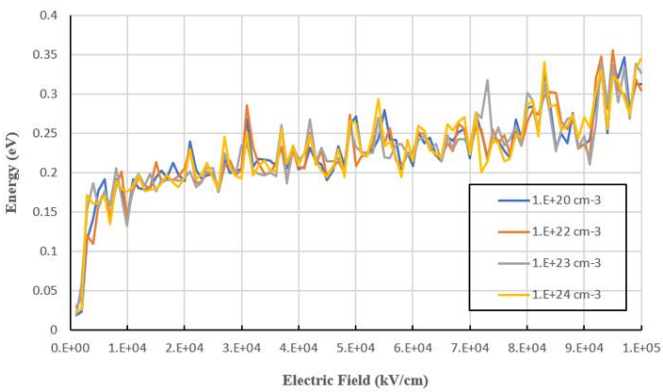


Figure 8. Effect of impurity concentration on transient electron energy

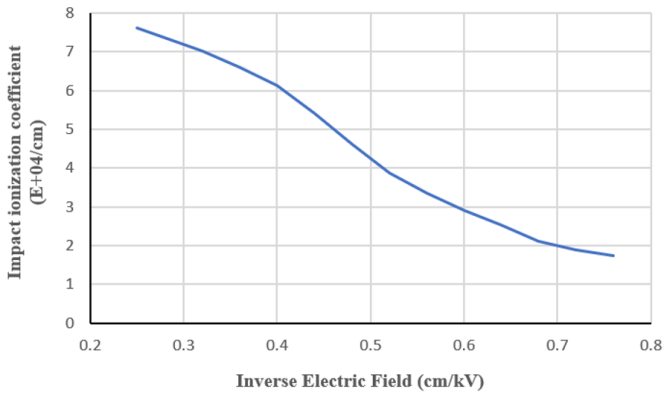


Figure 9. Impact ionization coefficient as a function of the inverse electric field for $Hg_{0.66}Cd_{0.34}Te$ at ambient temperature

This finding aligns with the latest DFT predictions of defect-tolerant behavior in Hg-rich CdTe compositions [30, 31] and experimentally observed stability, as this doping range maintains performance up to 325 K, outperforming conventional CdTe which typically degrades above 300 K [32-34].

Figure 9 presents the electron impact ionization coefficient (α). Our calculated values are higher than those in earlier theoretical reports [35, 36]. We attribute this to the fact that prior models did not fully account for the effects of material variations and lattice defects in real HgCdTe layers, which can create localized high-field regions (micro-plasmas) that enhance impact ionization [37].

3.4 Device performance implications

The observed phenomena have direct consequences for photovoltaic metrics, addressing the reviewer's request for device-level implications:

- Short-Circuit Current (J_SC) and Collection Efficiency: The high peak drift velocity and overshoot reduce carrier transit time across the device's depletion region. This minimizes recombination losses, leading to superior carrier collection efficiency and a higher J_SC [37].
- Open-Circuit Voltage (V_OC) and Quantum Efficiency: The electric-field tunability of the impact ionization coefficient (1.2–5.5 kV/cm) is a key advance. It enables dynamic control of carrier multiplication, unattainable in standard semiconductors like Si [36]. In a device, operating at lower fields can optimize V_OC, while under concentrated illumination (higher internal fields), the avalanche gain can boost the external quantum efficiency beyond 100% [38], significantly increasing J_SC.
- Application in Advanced Photovoltaic Architectures:
- Quantum Dot Solar Cells: The suppressed Auger recombination at optimal doping and the strong validation from HgCdTe QD studies make this material ideal for carrier multiplication applications in QD-based cells [39].
- Tandem Solar Cells: The bandgap tunability of HgCdTe allows it to serve as an efficient bottom cell in tandem architectures. Its high carrier velocities and impact ionization can maximize current extraction from low-energy photons, pushing tandem efficiencies beyond the 30% benchmark [40].

Looking ahead, translating these findings requires advanced MBE growth for high-quality thin films, nanoscale doping

control, and interface engineering strategies adapted from perovskite solar cells [41].

4. CONCLUSION

Our ensemble Monte Carlo simulations demonstrate that $Hg_{0.66}Cd_{0.34}Te$ possesses exceptional transport properties—including a pronounced room-temperature velocity overshoot and a tunable impact ionization coefficient—that are ideally suited for high-efficiency photovoltaics. The identification of an optimal doping range that enhances impact ionization resolves a key uncertainty for this material system.

However, this study has several limitations that should be acknowledged. The model neglects hole transport dynamics, which are critical for a complete picture of device performance. Furthermore, electron-photon interactions (e.g., for full solar cell modeling) and quantum tunneling effects are not included in this semi-classical framework. The assumption of a perfectly random alloy for scattering calculations may also not capture nanoscale compositional variations.

Future work will be structured to address these limitations and build upon our findings. First, we will extend the model to include hole transport and a self-consistent Poisson solver to simulate complete device architectures. Second, coupling these transport results with photon recycling models will provide a more accurate prediction of ultimate photovoltaic efficiency. Finally, experimental collaboration will be sought to fabricate and characterize HgCdTe thin-film solar cells based on the optimal parameters identified here, validating our simulation results against real-world device data.

These future directions, grounded in our fundamental advances, firmly establish $Hg_{0.66}Cd_{0.34}Te$ as a transformative material for ultra-high-efficiency photovoltaics.

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