

Atomistic Solution Carrier Field Mobility Characterization





FIELD MOBILITY CHARACTERIZATION



- Mobility modeling divided into: (i) low-field behavior, (ii) high field behavior, (iii) bulk semiconductor regions and (iv) inversion layers
- Calculate equilibrium conditions mobility
- Using some fitting parameters
- > Lot of Hits & Trials require
- Continuum Model's proposed by others



In reality, carriers accelerated by electric fields, lose momentum as a result of various scattering processes. These scattering mechanisms include lattice vibrations (phonons), impurity ions, other carriers, surfaces, and other material imperfections. Since the effects of all of these microscopic phenomena are lumped into the macroscopic mobilities introduced by the BTE equation these and are functions of the local electric field, lattice temperature, doping concentration, and so on.





TNL-EM SIMULATOR



Features

- Graphical User Interface (GUI) based
- □ Windows based application
- **Boltzmann transport equation solution**
- **□** Ensemble Monte Carlo Technique
- □ Include standard scattering mechanisms
- □ Fermi Golden Rule for momentum & energy conservation
- □ Modeled beyond the effective-mass approximation on the full electronic band structure obtained from FullBand Simulator
- □ The electron-phonon, electron-impurity, and electron-electron scattering rates included in a way consistent with the full band structure of the solid
- The carrier transport on the full energy band under influence of electromagnetic forces is traceable for each single carrier.
- □ Accurate up to a particle level





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The equation is given as

$$\frac{df}{dt} + \nabla_k E(k) \cdot \nabla_r f + F \cdot \nabla_p f = \left| \frac{df}{dt} \right|_{scattering} + GR$$

Here f is the distribution function, E is the electric field, F is the external electromagnetic force.

□ Solution of 6+1 dimensional is possible through:

> A spherical harmonic expansion (SHE) method with initial approximations

 \succ accuracy of simulation results ??

- > The ensemble Monte Carlo (EMC) technique (stochastic), to simulate non-equilibrium transport in semiconductor.
- > In Monte Carlo (MC) method, physics is more straightforward and provides flexibility in exploring physical mechanisms and carrier transport.





TNL-EM SIMULATOR







GROUP-III NITRIDES



solid lines represents – *TNL-EM Simulator* experimental results open circles, squares and triangles for AIN, GaN and InN respectively.

O'Leary, S. K., Foutzb, B. E., Shur, M. S., Bhapkar, U. V. & Eastmanb, L. F., Monte Carlo simulation of electron transport in wurtzite aluminum nitride, *Solid State Communications* 105, 621-626, (1998).
Marini, J., Bell, L. D. & Shahedipour-Sandvik, F. Monte Carlo simulation of III-nitride photocathodes. *J. Appl. Phys* 123, 124502(1-9) (2018).
Reklaitis, A. Nonequilibrium optical phonon effect on high-field electron transport in InN, *J. Appl. Phys.* 112, 093706(1-6) (2012)



* Scientific Reports, Nature Journal, 2020.











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- > ADVANCED LICENSING OPTIONS:
- Term-Based
- Perpetual
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Publications



- 1. P.K. Saxena, numerical study of dual band (MW/LW) ir detector for Performance improvement, *Defence Science Journal*, vol. 67(2), (2017) pp. 141-148. DOI : 10.14429/dsj.67.11177
- 2. Praveen K. Saxena, Pankaj Srivastava, R. Trigunayat, An innovative approach for controlled epitaxial growth of GaAs in real MOCVD reactor environment, Journal of Alloys and Compounds, vol. 809 (2019) 151752. https://doi.org/10.1016/j.jallcom.2019.151752
- 3. Praveen Saxena, R. Trigunayat, Anchal Srivastava, Pankaj Srivastava, Md. Zain, R.K. Shukla, Nishant Kumar, Shivendra Tripathi, FULL ELECTRONIC BAND STURCTURE ANALYSIS OF Cd DOPED ZnO THIN FILMS DEPOSITED BY SOL-GEL SPIN COATING METHOD, II-VI US Workshop Proceedings, 2019.
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- 5. Sanjeev Tyagi, P. K. Saxena, Rishabh Kumar, Numerical simulation of InxGa1–xAs/InP PIN photodetector for optimum performance at 298 K, Optical and Quantum Electronics (2020) 52:374. https://doi.org/10.1007/s11082-020-02488-1
- 6. A. Srivastava, A. Saxena, P. K. Saxena, F. K.Gupta, P. Shakya, P. Srivastava, M. Dixit, S.Gambhir, R. K. Shukla & A. Srivastava, An innovative technique for electronic transport model of group-III nitrides, *Scientific Reports* 10, 18706 (2020).
- 7. PK Saxena, A Srivastava, A Saxena, F Gupta, P Shakya, A Srivastava, et. al., <u>An Innovative Model for Electronic Band Structure Analysis of</u> Doped and Un-Doped ZnO, Journal of Electronic Materials 50 (4), 2417-2424(2021).
- 8. P. K. Saxena, F. K. Gupta, A. Srivastava, P. Srivastava1 and Anshu Saxena, Ultrafast carrier's dynamics with scattering rate saturation in Ge thinfilmsUltrafast carrier's dynamics with scattering rate saturation in Ge thinfilms TechRxiv · Mar 17, 2022







