Generation of III-Nitride Transport Parameters with *Mocasim*

Mocasim is an advanced three-valley Monte Carlo simulator designed to generate the transport parameters used in Silvaco's physical device simulators. It accurately calculates the material transport parameters of both direct and indirect band gap semiconductors, including group IV and III-V material systems. With the recent interest in III-Nitride material systems, we have added the capability of simulating materials with wurtzite as well as zincblende and diamond lattices. ***Mocasim*** derives a multi-dimensional parameter set, including mobility, velocity, energy and momentum relaxation times, and inter-valley potential energy, all of which can be extracted as a function of applied electric field, doping density, mole fraction(s), and lattice temperature.

Mocasim is a physically based simulator. As such, it has three major advantages over empirical modeling:

- It is predictive
- It provides insight
- It captures theoretical knowledge in a way that makes this knowledge easyto understand

Physically based simulation is different from empirical modeling. The goal of empirical modeling is to obtain analytic formulae that approximate existing data with good accuracy and minimum complexity. Empirical models provide efficient approximation and interpolation. They do not provide insight, predictive capabilities, or encapsulation of theoretical knowledge. Physically based simulation is an alternative to experiments as a source of data. Empirical modeling can provide compact representations of data from either source.

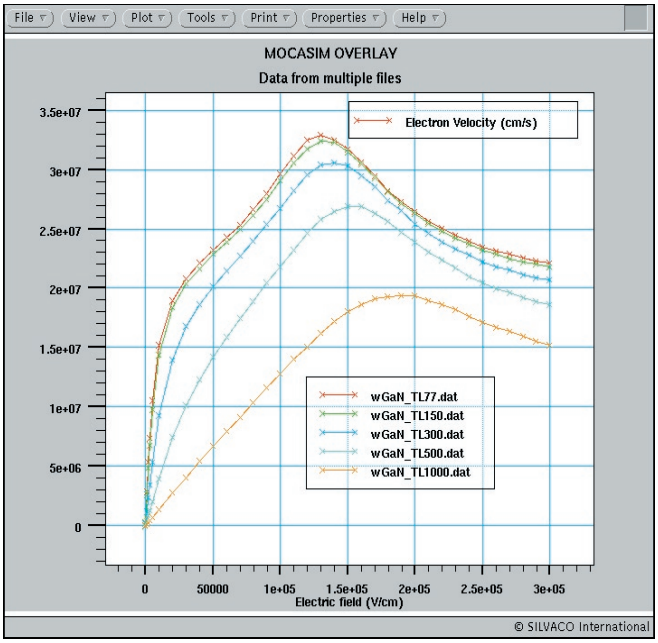

Figure 1. ***Mocasim*** generated curves of electron velocity versus electric field for wurtzite GaN at different ambient temperatures.

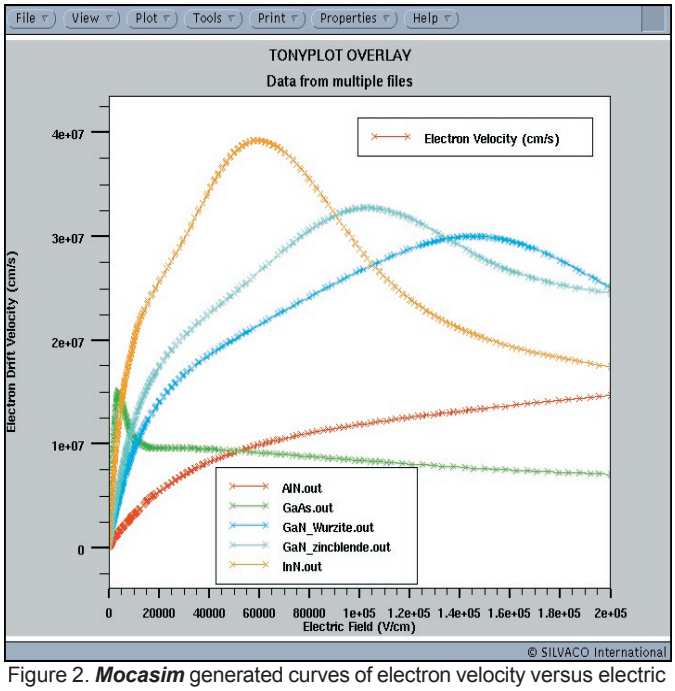

Figure 2. ***Mocasim*** generated curves of electron velocity versus electric field for GaAs, AnN, InN, wurtzite GaN and zincblende GaN.

Physically based simulation has become important for two reasons: First, it is almost always much quicker and cheaper than performing experiments. Second, it provides information that is difficult, or impossible to measure. These advantages are of special interest in the case of III-Nitride materials, which can be difficult to manufacture and measure.

There are drawbacks as well to physically based simulation. The drawbacks are that all the relevant physics must be incorporated into the simulator, and numerical procedures must be implemented to solve the associated equations. These tasks have been taken care of for users of ***Mocasim***. Physical scattering mechanisms built into ***Mocasim*** include scattering from polar and non-polar optical phonons, deformation potential acoustic phonons, piezo-electric acoustic phonons, ionized or neutral impurity scattering, and inter-valley phonon scattering.

Parameter	z-GaN	w-GaN	w-AlN	w-InN
Lattice	Zincblende	Wurzite	Wurzite	Wurzite
Density(g/cm3)	6.15	6.15	3.23	6.81
Longitudinal Speed of Sound (x1e5 cm/s)	4.57	6.56	9.06	6.24
Static Dielectric Constant	8.90	8.90	8.50	15.30
RF Dielectric Constant	5.35	5.35	4.77	8.40
Effective Masses				
Valley 0	0.150	0.190	0.480	0.110
Valley 1	0.400	0.400	1.000	1.000
Valley 2	0.600	0.600	1.000	1.000
Bandgap (eV)				
Valley 0	3.40	3.50	6.20	1.89
Valley 1	4.70	5.50	6.90	4.09
Valley 2	6.00	5.60	7.20	4.49
Non-Parabolicity (1/eV)				
Valley 0	0.213	0.183	0.044	0.419
Valley 1	0.065	0.065	0.000	0.000
Valley 2	0.029	0.029	0.000	0.000
Degeneracy				
Valley 0	1(G)	1(G)	1(G)	1(G)
Valley 1	3(X)	6(L-M)	6(L-M)	1(A)
Valley 2	4(L)	1(G')	2(K)	1(K)
Polar Optical Phonon Energy (meV)	91.20	91.20	99.20	89.00
Acoustic Deformation Potential (V)	8.30	8.30	9.50	7.10

Table 1. Basic set of material parameters used in the ***Mocasim*** velocity - field simulations for zincblende GaN and wurtzite GaN, AlN, and InN.

In the case of new materials, however, there is also the need to find the relevant parameters associated with these mechanisms. We have done a literature search 1-4 and assembled in Table 1. some of the needed parameters for wurtzite GaN, AlN, and InN, as well as zincblende GaN. This enables, through the appropriate interpolation routines, the parameters for ternary or quaternary materials from the binary parameters. Although there is not yet a consensus on precise values of these parameters, our simulations of electron velocity versus electric field with doping and temperature as parameters, as shown in Figure 1 and Figure 2, have been compared with measurements and other (non-commercial) simulations found in the literature with consistent results. Our Figure 1 can be compared with Bhapkar's Figure 1a for electron velocity vs field for wurzite GaN with Nd=1e17 cm-3 for a range of temperatures: T=77, 150, 300, 500, and 1000K. Our Figure 2 shows electron velocity vs field for GaAs, InN, AlN, and GaN in both zincblend and wurzite forms. Compare with Faramond5 for wurzite GaN, InN, and AlN; Figure 2 in Kolnik4 for wurzite and zincblende GaN; and Foutz3 for GaAs and GaN.

References

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