Mocasim – A Versatile Monte Carlo Simulator for III-Nitride Transport Properties

III-Nitrides have recently attracted attention as a promising material class for high-power, high-frequency microelectronic applications at elevated temperatures. They possess large band gaps, relatively small effective masses in the conduction band minimum, large offsets to the conduction band satellite valleys, and high polar optical phonon frequencies. The large band gaps provide high-breakdown field strengths, while the other basic physical properties result in high low-field mobilities and high saturation velocities.

Monte Carlo Generated Materials Transport Parameters

For this report, we utilized the ***Mocasim*** Monte Carlo simulator to derive carrier velocity characteristics for common III-Nitride binaries and their ternary alloys ($Al_xGa_{1-x}N$, $In_xGa_{1-x}N$, and $Al_xIn_{1-x}N$ in their wurtzite phase). Material model parameters are derived as a function of field, doping, mole fraction, and temperature. The example in Figure 1 shows the electron velocity as a function of electric field strength for $Al_xGa_{1-x}N$ at room temperature.

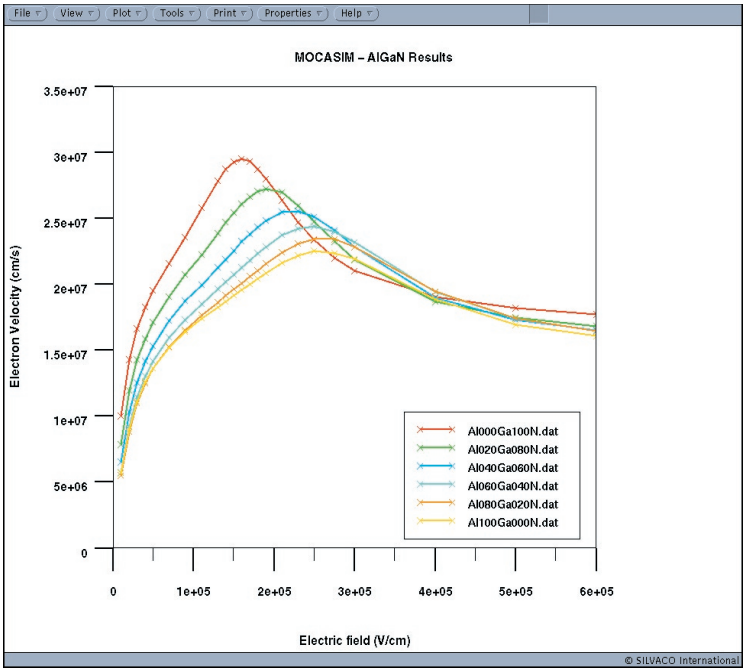

Figure 1. Electron drift velocity in bulk $Al_xGa_{1-x}N$ as a function of electric field strength at room

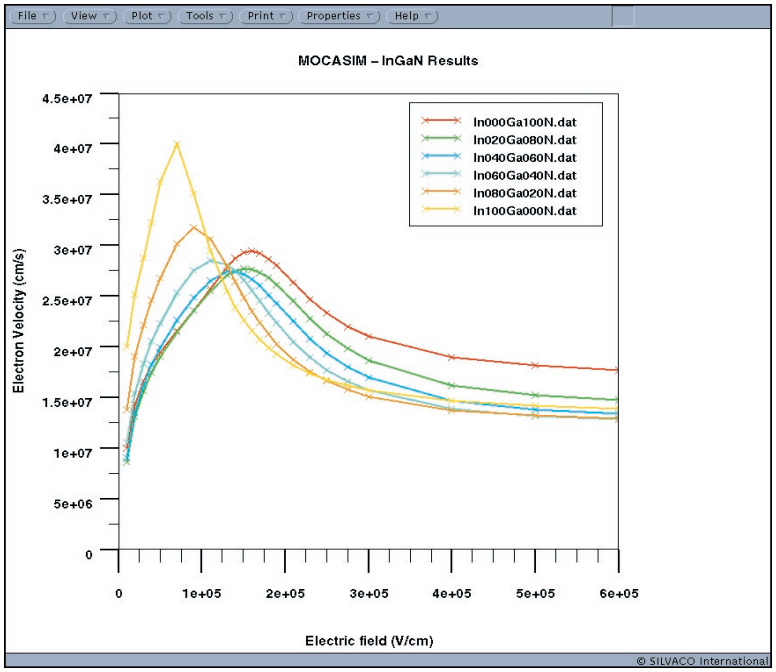

Figure 2. Electron drift velocity in $In_xGa_{1-x}N$ as function of electric field strength for various alloy concentrations x at room temperature.

Energy, momentum relaxation times, and other basic transport parameters that form the physical basis for advanced ***FastBlaze*** energy balance simulations are also calculated from ***Mocasim*** as a function of carrier energy, doping, mole fraction and temperature. These quantities, calculated directly from band structure data and all relevant scattering mechanisms, provide an accurate representation of velocity overshoot and non-local transport effects within ***FastBlaze*** energy balance simulations.

Drift Velocities in III-Nitrides

$Al_xGa_{1-x}N$ alloys are the materials most widely used in the fabrication of III-Nitride FETs. The drift velocities of electrons as a function of electric field strength in this material family are depicted in Figure 1 for various alloy concentrations x. Starting from $Al_xGa_{1-x}N$ with x=0, a decrease in low field drift mobility as well as a decrease in peak-velocity with increasing Al content is observed. Both effects are primarily

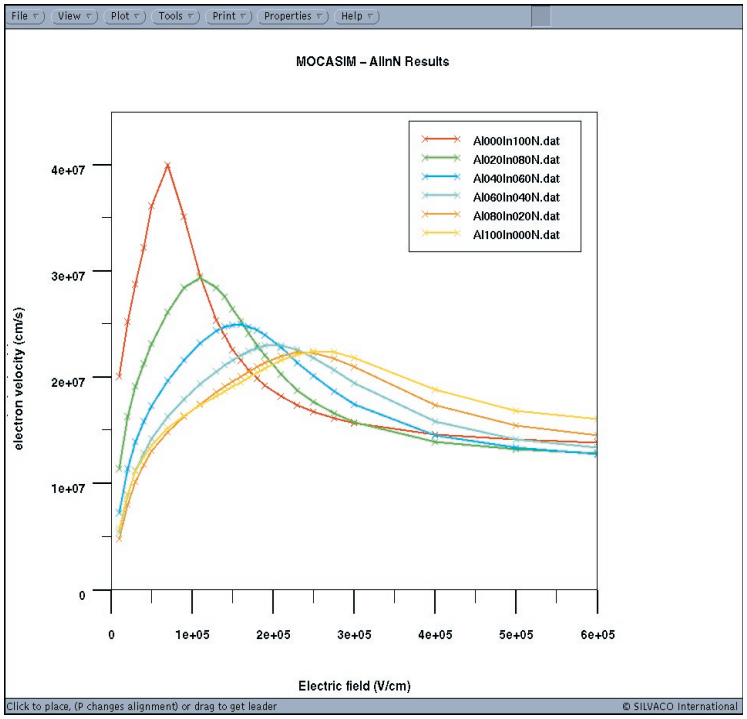

Figure 3. Electron drift velocity in $Al_xIn_{1-x}N$ as function of electric field strength for various alloy concentrations x at room temperature.

a direct consequence of the increasing effective mass of the central valley. The saturation drift velocities, on the other hand, remain nearly constant over the entire range from one binary to the other.

InN contains the smallest effective mass of the three binaries (GaN, AlN and InN), so that InGaN channel FETs are considered as a candidate for very high frequency applications. To exploit the potential of the $In_xGa_{1-x}N$ alloy in terms of mobility and drift velocities, we performed ***Mocasim*** calculations of this material family. In contrary to the alloys $Al_xGa_{1-x}N$ and $In_xAl_{1-x}N$, the favorable influence of the decreasing effective mass of the alloy is overcompensated by the increasing influence of $In_xGa_{1-x}N$ alloy scattering. This results in a decrease of the low field mobility as well as the peak drift velocity by increasing the In content up to about 40%.

A simplified version of a tight binding-based model [1] that is similar to the standard model [2,3] for alloy scattering was implemented for this study. ***Mocasim's C-interpreter*** Capability was used in order to implement user-defined scattering mechanisms. The saturation velocity is reduced primarily as a result of the lower energetic separation of the satellite valleys from the central conduction band minimum. A slightly higher deformation potential also enhances this effect. Despite the negative transport features of $In_xAl_{1-x}N$, the additional degree of freedom for band profile engineering originates in the high polarization induced fields in layered structures. InxGa1-xN remains a promising alloy for MODFET applications.

$Al_xIn_{1-x}N$ displays a similar, but less pronounced behavior for the drift velocities of electrons than is otherwise found in $In_xGa_{1-x}N$. The low field mobility decreases slightly, with an increase of In content that results from scattering due to alloy fluctuations. This overcompensates for the effect of the decreasing effective mass in the central conduction band minimum. For the same competing mechanisms, peak velocity remains almost constant for In contents up to 20%, while steadily increasing for higher In concentrations. The threshold field to the regime of negative differential mobility, on the other hand, monotonically shifts to smaller field values by increasing the In content of the alloy. This is a consequence of the decreasing effective G-valley mass and the decreasing energetic separation to the satellite valleys. The saturation velocities are reduced for the same reasons as for InxGa1-xN with increasing In content, whereby alloy scattering results in a lowering of the saturation drift velocity for intermediate alloy concentrations.

Another key property of nitrides is that they possess large spontaneous, piezoelectric polarization fields that induce high channel densities in HFETs without doping. Such polarization fields are added to ***FastBlaze*** HFET simulations by including fixed sheet charges that are induced by the abrupt change of pyro- and piezoelectric polarization at the heterointerfaces.

References

[1] P. A. Fedders and C. W. Myles, Phys. Rev. B 29(2), 802 (1984)

[2] J. W. Harrison and J. R. Hauser, J. Appl. Phys. 47(1), 292 (1976)

[3] M. Fahramand et al., IEEE Trans. On Electron Dev. 48(3), 535 (2001).