

# MOCASIM – Monte Carlo Transport Parameter Generator

Andrew Plews & Robert Drury

SILVACO International  
4701 Patrick Henry Drive, Santa Clara, CA 95054

Modern physical device simulators require a wide range of both material and bias-dependent transport parameters. Even for the simplest of mobility models the availability of published data becomes questionable once the user moves away from common material systems. Further, even if mobility is characterized (usually only over a limited range) users also require additional relationships to implement the advanced hydrodynamic transport models necessary to accurately describe modern devices. These relationships are often completely unavailable for more exotic material systems.

Therefore, to provide the transport parameters for SILVACO's range of physical device simulators, we created MOCASIM, a new physical transport parameter simulator. MOCASIM has been designed to generate material dependent transport parameters for both direct and indirect band gap cubic semiconductors - including group IV and most of the group III-V material systems (Figs. 1 & 2).

MOCASIM is a three-valley ensemble Monte Carlo simulator that generates the non-equilibrium carrier distribution function by directly modeling the transport processes in an ideal crystal. Carriers initially start with energy distribution given from equilibrium Boltzmann statistics at the ambient lattice temperature. They then undergo acceleration by an applied electric field and are scattered into different states through a variety of different mechanisms. This process is repeated, typically tens of millions of times, until the new carrier distribution reaches steady state. Finally, the transport parameters are extracted by performing an ensemble average over the new distribution.

MOCASIM has been designed to be flexible, allowing the user to specify an arbitrary number of scattering mechanisms to efficiently simulate different materials. These processes may be selected from a library of predefined scattering mechanisms or be completely user-defined through the SILVACO C-INTERPRETER. Further, the user controls the majority of the simulation parameters including the number of samples, energy ranges, burn-in time (Fig. 3) etc.

Finally, MOCASIM derives a multi-dimensional parameter data set, including mobility, velocity (Fig. 4), energy and momentum relaxation times and inter-valley potential energy, all of which can be extracted as a function of applied electric field, net impurity density, mole fraction(s) and lattice temperature.

For a review of MOCASIM and all other SILVACO products go to our home page at : <http://www.silvaco.com>

Fawcett W., Boardman A.D. and Swain S., "Monte Carlo Determination of Electron Transport Properties in Gallium Arsenide", J. Phys. Chem. Solids, Periamon Press 1970, Vol. 31, pp. 1963-1990

Jacoboni Carlo and Reggiani Lino, "Bulk Hot-Electron Properties of Cubic Semiconductors", Advances in Physics, 1979, Vol. 28, No. 4, pp. 493-553

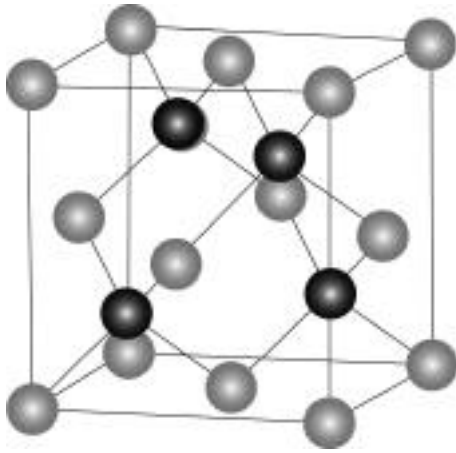


Figure 1. Group III-V material zincblende crystal structure. Note: Group IV materials have the same structure, however all the atoms are identical

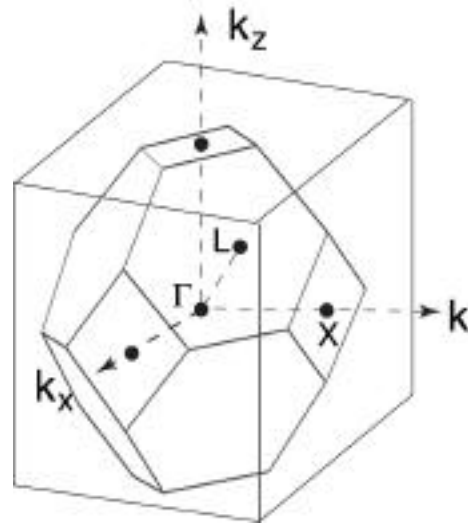


Figure 2. First Brillouin zone of the face-centered cubic lattice showing directions of high symmetry.

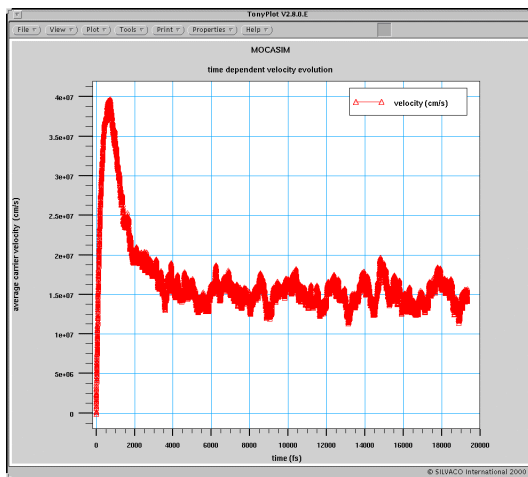


Figure 3. Evolution of the average carrier velocity over a typical MOCASIM run. This figure illustrates the “burn-in” time associated with the simulation, where the carriers are redistributing from the initial non-equilibrium to final states.

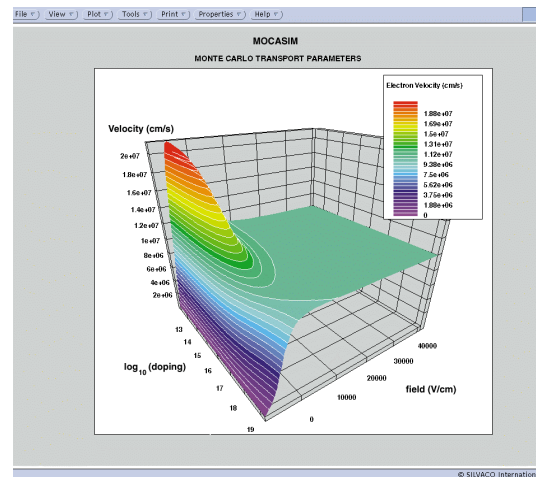


Figure 4. The electron velocity surface for GaAs at 300K as a function of net impurity density and electric field