Using The Statistical Sampling Feature in Silvaco's BCA Monte Carlo Implant Simulator

1.0 Introduction

Silvaco's Binary Collision Approximation (BCA) Monte-Carlo Implantation simulator closely replicates the physics of implantation by individually tracking implanted ions and their resulting interstitial and vacancy damage as the ions collide and interact with atoms in the substrate. The simulator then tracks subsequent ions, gradually building up the implanted ion concentration profile, until the required number of ions is reached.

All implanted ions do not come to rest at the same depth in the substrate due to different interaction with the substrate atoms. An implanted ion that collides head on with a substrate atom at the surface is more likely to come to rest closer to the surface than an implanted ion that channeled between atoms for some distance before colliding head on with an atom.

There is a statistical probability that some implanted ions travel relatively long distances between substrate atoms without encountering a collision event. This is especially true in an ordered structure such as a silicon crystal. On rare occasions, the eventual collision of the travelling ion results in another trajectory that allows a relatively long flight path before another collision. The few implanted ions that travel very deep into the substrate are usually the result of several rare events. Despite their relative rarity, however, the vast amount of implanted ions ensure that even rare events affect the overall implanted profile and must be taken into account.

The graph of a low-energy arsenic implant (Figure 1) illustrates how rare events affect the implantated profile. The few straggling ions that penetrated deepest into the substrate represent these events. If the number of simulated ions were equal to the number of ions actually implanted, these statistical aberrations would accurately reflect reality. Time constraints typically limit the number of simulated ions, however, so each are weighted accordingly. This has a minimal effect on accuracy apart from these rare events, which are considered statistical aberrations at the "tail end" of the implant. If more ions are implanted than simulated, the concentration in the tail of the implant would be smoother in reality than in the simulation. To correct for this, a new algorithm has been implemented in ATHENA. The algorithm is invoked by the "sampling" parameter in the "implant" statement.

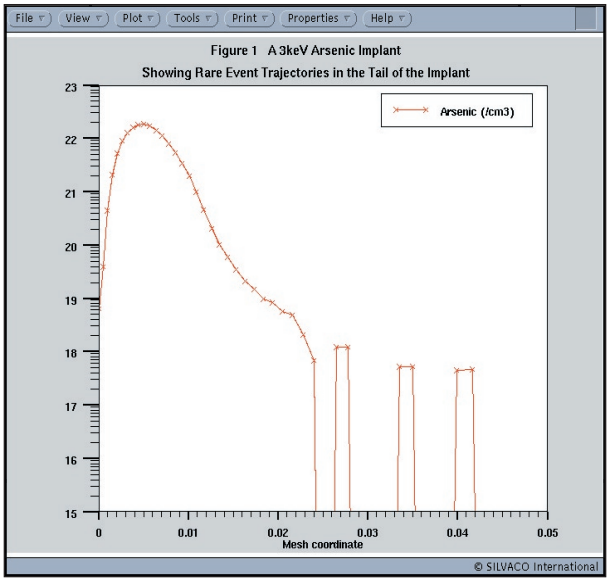

Figure 1. A typical Monte-Carlo simulation of a 3 keV Arsenic implant showing rate event ion trajectories in the tail of the concentration profile.

2.0 Implementation of the Rare Event Correction Algorithm

ATHENA reduces calculation time and improves statistical quality of simulated profiles by means of a three-dimensional rare event algorithm. An implantation profile often differs significantly in concentration value across implantation depth. Low concentrations in the profile are due to the low probability of implanted species (rare events) to reach that point in space. A valid statistics profile is comprised of a number of simulated cascades that are relative to the desired level of accuracy. Depending on device size, implant distributions below a certain threshold concentration value may exhibit significant statistical noise, even in real experiments.

The algorithm uses trajectory splitting to achieve an increased occurrence of rare events by generating several independent sub-trajectories from more common events. The original idea, [1], was first developed into a refined simulation technique by Villién-Altamirano et al., [2]. Their version of this approach is called "restart." The basic idea is to identify subspaces from which it is more likely to reach the rare event's target subspace. Each time these subspaces are reached, current event sequences are split into a number of replicas, all continuing forward from a state of splitting. In this way the number of rare events increase, depending on the number of restart thresholds defined and the amount of replicas generated.

The trajectory-splitting algorithm naturally fits into the problem of Monte Carlo simulation of stopping and ranges, such as ion implantation. A similar method was first used in the work of Phillips and Price, [3], to simulate hot electron transport. The first rare event algorithm that applied to the transport phenomena simulation of ions in matter was used by Yang et al., [4]. Later, Beardmore et al., [5], significantly refined the rare event algorithm. A brief, but comprehensive review of trajectory splitting methods used in modeling of ion implantation is given in [6].

The increased speed of the rare event trajectory splitting technique is due to changes in the statistical behavior that provoke rare events to occur more frequently. ***ATHENA's*** rare event algorithm achieves this by identifying likely subspaces from which to observe a given collision event, and then making replicas of the cascade sequences that reach those subspaces. Figure 2 illustrates the trajectory splitting and the restart of replica events as a new threshold is reached. When applying splitting to collision cascades, or other specific system, the two main parameters to determine are: first, when to split and, second, how many sub-trajectories to create when splitting.

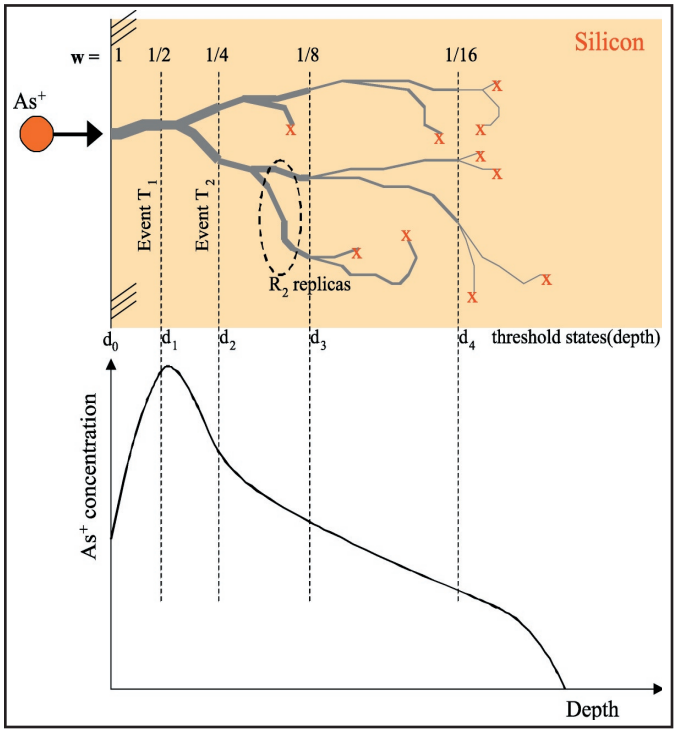

Figure 2. Restarting collision events by splitting at 'm' thresholds.

Different criteria are used to obtain the threshold states when splitting must occur. For example, Bohmayr et al., [7], use a trajectory split method based upon checking the concentration of local dopant molecules at certain points. Beardmore, et al's. rare event algorithm, [5], uses the integrated dose as a criterion for deciding when to split. ***ATHENA*** uses the same criterion to determine the splitting depths. Dose integration is carried out along the radius vectors of ions' co-ordinates, thus, roughly taking into consideration the three-dimensionality of the ion distribution.

Due to the discrete nature of collision cascades, the number of sub-trajectories created at each split depth should be an integer greater or equal to two. Let T i i represent the event at each threshold state (the event of an ion passing through a split depth). The probability of an ion in state T i-1 i-1 to reach T i i state is pi = P(T i i |T i-1 i-1) 1) . Then the recommended number of replications at each threshold (a split depth) is Ri=1/ pi. This relation links the number of replications at each split and the criterion necessary to identify the threshold states (split depths). If Ri=2, then the number of ions passing through split depth, d i i , will be twice smaller than the number of particles passing through split depth d i i . ATHENA's criterion to determine the split depths is the integrated dose along the radius vectors of stopped particles. For example:, split depths d i i , d 2 2 , d 3 3 , etc. will be at integrated doses 0.5Φ , 0.75Φ , 0.875Φ , etc. where Φ is the total retained implant dose.

In ***ATHENA***, trajectory splitting is turned on with the sampling command in the implant statement. In theory, sampling estimators are unbiased and consistent, as theoretical expectation is obtained from the whole ensemble of sample paths, including very unlikely ones. In practice, the estimate is obtained as the average of finite number of samples. Overbiasing can occur if the only goal is to increase the probability of the event that requires further analysis. Overbiasing usually results in the underestimation of the evaluated probability (dopant concentration, in case of ion implantation). In fact, it has been reported in [8] that when the splitting

parameters are not consistent with the system's large deviations behavior, the probability in question may be severely underestimated. This situation is almost present in ion implant simulators when treating multi-layered targets and two-dimensional layouts. Therefore, splitting should be used with caution. In conclusion:

- Variance reduction is not guaranteed by an increased occurrence probability of the event pending analysis.
- Trajectory splitting should be used carefully. Complex implantation geometry can lead to considerable system behavior deviation, thus overbiasing and underestimating the relevant statistics.

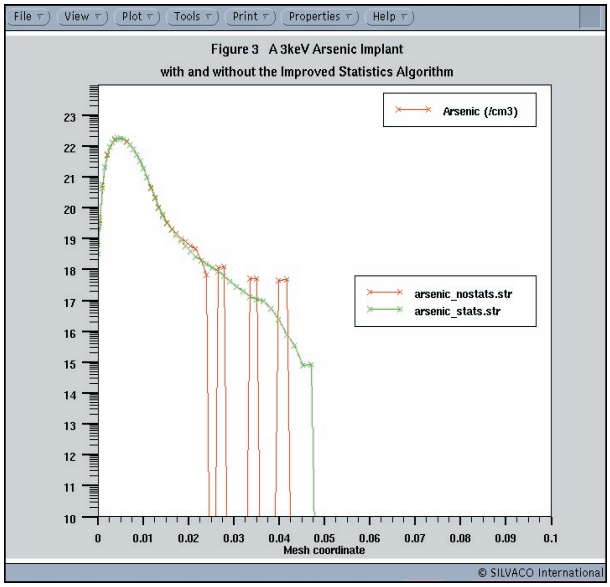

Figure 3. A 3keV Arsenic Implant at 7 degrees from vertical with and without the new statistical algorithm activated.

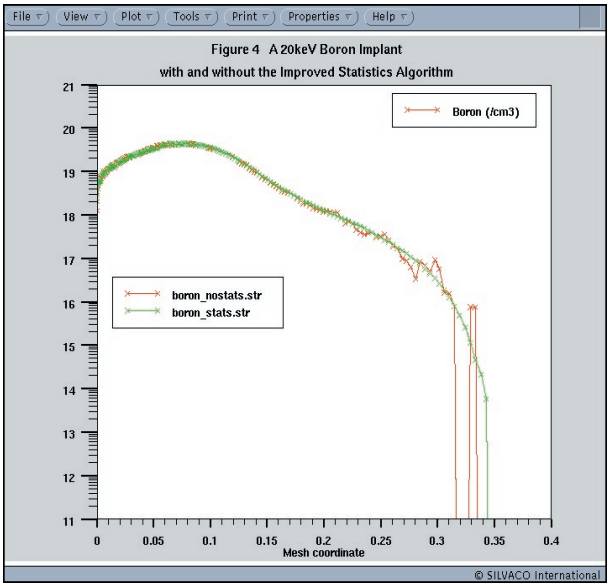

Figure 4. A 20keV Boron Implant at 7 degrees from vertical with and without the new statistical algorithm activated.

3.0 Results and Examples

Typical results showing the improved statistics encountered when using the "sampling" parameter on the Monte-Carlo implant statement are shown in figures 3 and 4. Both figures show typical implant curves with and without the "sampling" parameter activated. The improvements in smoothness at the tail of the implant profiles are clear. All simulations used the same number of ion trajectories. These improvements, therefore, are solely the result of improved statistics using the new algorithm.

References

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