Stable simulation of impurity fluctuation for contact resistance and Schottky diodes

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Abstract

The influence of the discretized impurity distribution on transport at Schottky contacts is stably simulated with the long-distance component of the Coulomb potential. The present approach suppresses the artificial fluctuation of the impurity density. We can avoid the extremely high conduction and the dependence on the grid distance around contacts. The standard deviation of the contact resistance is expected to be about 10% for small areas, and the worst standard deviation appears around a donor density of 10^{18} cm^{-3} for CoSi$_2$ contacts.

1 Introduction

The electrical characteristics between metal and semiconductor are becoming critical issues limiting the performance of devices. Examples of such issues include the triggering of ESD protection devices for low-voltage operation, immunity to short channel effects in Schottky transistors, and contact resistance in deca-nano-scale devices. This paper presents stable simulation results of the effects of a discretized impurity distribution on the contact resistance and Schottky diodes. A unified simulation based on the Schottky contact model [1] was used to analyze these effects.

2 Simulation method

Figure 1 shows the potential profiles formed by a Schottky barrier and the discretized impurities for a donor density N_D of 10^{20} cm^{-3}. An impurity sited near the barrier makes the tunneling potential steep in regions where the current density is concentrated. Therefore, the treatment of the potential around discretized impurities is important in the evaluation of the influence of impurity fluctuations on the electrical characteristics. Figure 2 shows the typical rectifying characteristics of a Schottky barrier diode (SBD) with $N_D = 10^{18}$ cm^{-3}. The current density fluctuates significantly under reverse bias conditions. This fluctuation may have a negative influence on the Schottky transistor and the trigger diode of the ESD protection device. The average value of the reverse currents with the bare impurity potential appears to be higher than that with the uniform distribution. This is because some highly conductive portions exist in the simulation using the bare potential of the impurities, and these portions dominate the reverse currents. Therefore, we adopted an approach of separating the short and long-distance components of the Coulomb potential in three-dimensional device simulation [2]. Figure 3 shows the long-distance component of an ionized impurity atom. The magnitude of the cut-off parameter ***kc*** is given by the inverse of the mean separation of impurities. Using the bare potential, extremely high donor densities appear around the contact as shown on the left in Fig. 4. This is because fine mesh arond the contact is nessesary to calculate the tunneling current of the Schottky barrier. The impurity density is inversely proportional to the grid distance under conditions in which the number and portions of impurity atoms are fixed. Whereas using the long-distance component effectively eliminates the extremely steep potential as shown on the right in Fig. 4. It is found that the results with the long-distance component fluctuate around those with the uniform distribution as shown in Fig. 2.

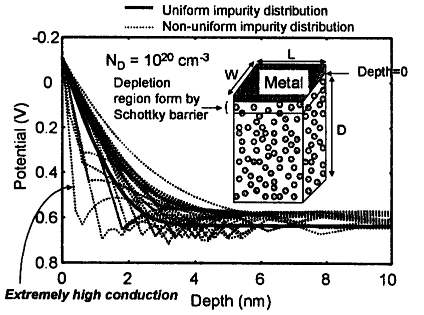

Figure 1: Potential profiles formed by a Schottky barrier and discretized impurities. The inset is a schematic of the locations of the discretized impurities.

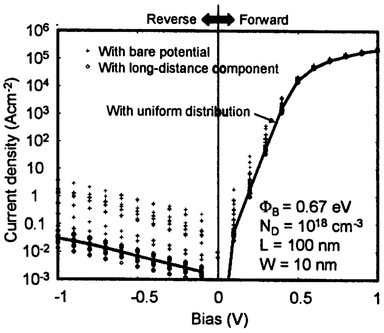

Figure 2: Rectifying characteristics of an SBD with $N_D = 10^{18}$ cm^{-3}.

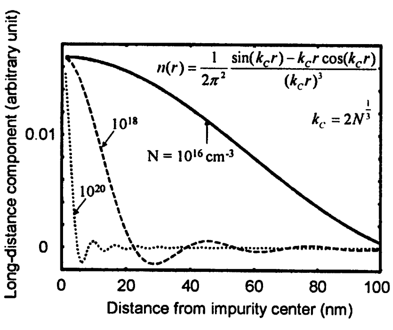

Figure 3: Long-distance component of an ionized impurity atom.

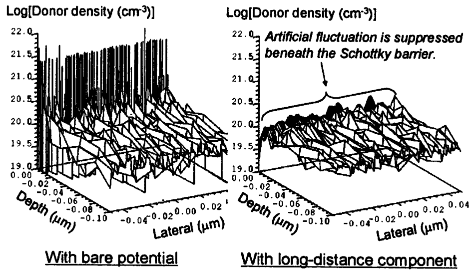

Figure 4: Potential profiles around Schottky contact.

3 Simulation results

Figure 5 shows the grid distance dependence of the average values of the contact resistance for ten kinds of randomized impurity distributions. Significant dependence appears when the bare potential is used. The anomalous increase in the small grid distance region is due to the traps of electrons around the bare potential of the impurity atoms. On the other hand, the grid distance is suppressed in the results obtained using the long-distance component. Figure 6 shows that the grid distance dependence of the normalized standard deviation of the contact resistance is also suppressed by using the long-distance component. It is expected that the standard deviation could be about 10% for $CoSi_2$ with $\Phi_B = 0.67$ eV. It is important to provide stable results as tools for engineering.

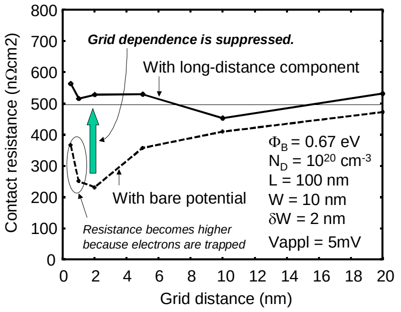

Figure 5: Grid distance dependence of the average contact resistance.

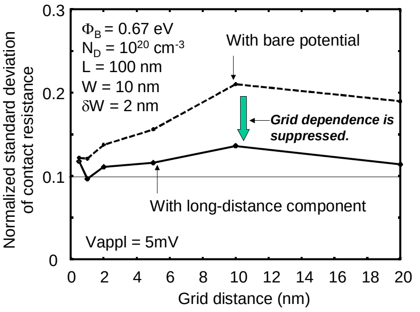

Figure 6: Grid distance dependence of the normalized standard deviation of contact resistance.

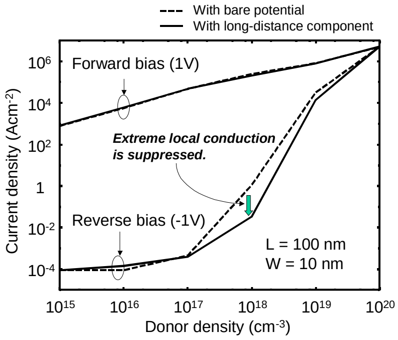

Figure 7: Impurity density dependence of the average of the reverse and forward currents of SBDs.

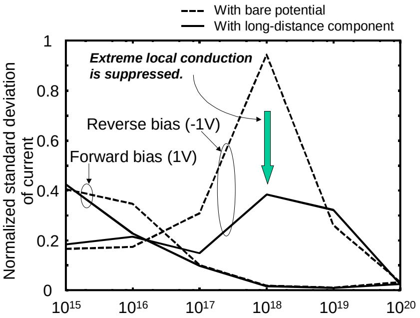

Figure 8: Impurity density dependence of the normalized standard deviation of the reverse and forward currents of SBDs.

Figure 7 shows the impurity density dependence of the average of the reverse and forward currents of SBDs. In agreement with the results in Fig. 2, extremely high conduction at 10^{18} cm^{-3} is suppressed in the results with the long-distance components.

Figure 8 shows the impurity density dependence of the normalized standard deviation of the reverse and forward currents. A peak appears in the reverse bias characteristics. In the low-density region, the fluctuation decreases as the density decreases, because the depletion region spreads and the whole currents become insensitive to the sites of the impurities. On the other hand, in the high-density region, the potential distribution formed by each impurity is averaged as the density increases. Therefore, the worst the standard deviation is expected to appear around a donor density of 10^{18} cm^{-3} for $CoSi_2$ contacts. The peak value becomes almost 100% for the bare potential, whereas the value obtained for the long-distance component is smaller. This is because the local high conduction is suppressed in the result with the long-distance component. The standard deviations for the forward bias conditions decrease monotonically as the density increases because the fluctuation of the impurities outside the depletion region is dominant.

4 Summary

The influence of discretized impurities on the transport between metal and semiconductor was simulated. It was found that simulations with the long-distance component of each impurity potential could provide a stable basis for prediction. When the long-component model is used, the standard deviation of the contact resistance is expected to become about 10% for $CoSi_2$. The impurity density dependence of the standard deviation shows a peak value around a donor density of 10^{18} cm^{-3}.

References

[1] K. Matsuzawa, K. Uchida, and A. Nishiyama, "A unified simulation of Schottky and ohmic contacts," IEEE Trans. Electron Devices, vol. 47, no. 1, pp. 103-108, 2000.

[2] N. Sano, K. Matsuzawa, M. Mukai, and N. Nakayama, "On discrete random dopant modeling in drift-diffusion simulations: physical meaning of ‘atomistic’ dopants," Microelectronics Reliability, vol. 42, pp. 189 -199, 2002.