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Simulation of interface states effect on the scanning capacitance microscopy measurement of \( p-n \) junctions

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A two-dimensional numerical simulation model of interface states in scanning capacitance microscopy (SCM) measurements of \( p-n \) junctions is presented. In the model, amphoteric interface states with two transition energies in the Si band gap are represented as fixed charges to account for their behavior in SCM measurements. The interface states are shown to cause a stretch-out and a parallel shift of the capacitance–voltage characteristics in the depletion and neutral regions of \( p-n \) junctions, respectively. This explains the discrepancy between the SCM measurement and simulation near \( p-n \) junctions, and thus modeling interface states is crucial for SCM dopant profiling of \( p-n \) junctions. © 2002 American Institute of Physics. [DOI: 10.1063/1.1532547]

Scanning capacitance microscopy (SCM) has been developed as a powerful dopant profiling tool of semiconductor devices on the submicron scale. To extract the dopant profile from SCM data, physical models are needed, because what is being detected in practice is approximately \( dC/dV \), the rate of change of the metal-oxide-semiconductor capacitance comprising the SCM probe and the underlying semiconductor with the ac bias between the sample and the SCM probe, \( V_{ac} \). So far, several models based on calibration methodology and nonjunction samples have been established and successfully applied to extract dopant profiles in neutral regions.\textsuperscript{1,2} Near \( p-n \) junctions, however, the dopant profiles determined by these models are invalid.\textsuperscript{3,4} A variant method for junction delineation has been proposed by Edwards et al.\textsuperscript{5} In this method, \( dC/dV \) is measured as a function of the dc bias \( V_{dc} \) between the sample and the SCM tip by cycling the \( V_{dc} \) in the experiment. The local \( C-V \) curves in the vicinity of a \( p-n \) junction can then be obtained by integrating \( dC/dV \), and thus the junction can be localized inside a narrow region (±30 nm). However, while this method gives a qualitative delineation of \( p-n \) junctions, so far, no quantitative dopant profiles of \( p-n \) junctions have been extracted using this approach. In our opinion, this is due to a lack of theoretical models that take into account the physics of SCM measurements near the \( p-n \) junction. This paper presents a two-dimensional numerical simulation model of interface states in SCM measurements of \( p-n \) junctions.

To account for the \( V_{dc} \) dependence of SCM output across \( p-n \) junctions,\textsuperscript{6,7} the experimental peak SCM output was used as the target data in our simulation. The peak SCM output was captured by sweeping the \( V_{dc} \) in the experiment using a DI Dimension 5000 system. The measurements were performed in spatial intervals of 0.1 \( \mu m \) across a one-dimensional silicon \( p^+ \)–\( n \) junction with an \( n \)-type substrate of uniform dopant density of \( 3 \times 10^{17} \) cm\(^{-3} \). The sweeping range of \( V_{dc} \) was set wide enough to cover both the positive and negative peaks of the SCM output across the junction to account for different flatband voltages at each spatial point.\textsuperscript{5}

Figure 1(a) shows the experimental peak SCM output versus position, \( x \) (solid line), with \( x=0 \) set at the \( p^+ \) edge. The data is normalized using the peak SCM output of the substrate.

This measurement was first simulated using a two-dimensional numerical model, which is interface states free.\textsuperscript{9} In this model, the Poisson and Laplace equations are solved. The carrier continuity equations are also solved to account for the response, to the SCM testing signals, of the minority carriers coming across the \( p-n \) junction in the measurement. The SCM probe is modeled as an infinite truncated blade.

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FIG. 1. (a) Normalized peak \( dC/dV \) data of the experiment (solid line) and the numerical simulation (open circles). The dashed line gives the extracted dopant profile corresponding to the simulation peak \( dC/dV \) data. (b) Schematic of the SCM interface states model. The energy distribution of the interface states is given in the inset of Fig. 2(a).
probe resting on the surface of the oxide layer that covers a $p-n$ junction. Various parameters of the SCM setup are modeled according to what occurred in practice (e.g., oxide thickness, width, and apex half angle of the SCM tip are 8 nm, 10 nm, and 17°, respectively). A $p-n$ junction dopant profile is extracted by repeatedly adjusting it until the difference between the normalized experimental and simulated peak $dC/dV$ data becomes as small as possible. The dopant profile extracted and its corresponding theoretical peak $dC/dV$ are also shown as a dashed line and open circles, respectively, in Fig. 1(a).

We can see from Fig. 1(a) that, in the neutral regions ($x<1.5$ and $x>2.2$ μm), the experimental and the simulation data match very well. However, near the junction (1.5 < $x$ < 2.2 μm, where the local C–V curves look like low-frequency C–V plots and give both positive and negative $dC/dV$ peaks), the simulated peak $dC/dV$ displays an opposite trend to the experimental data; that is, the former increases while the latter decreases as the SCM tip approaches the $p-n$ junction. Similar results can be found in other published data.

This discrepancy between the experimental result and the simulation motivated our investigation into interface states effect on SCM measurements, because although it is widely accepted that interface states distort the C–V curves, their specific effects in SCM still remain unclear. Our investigation of interface state effects was done through the following method. Firstly, interface states of an assumed energy distribution were introduced into the earlier model on the Si–SiO$_2$ interface. We assumed the energy distribution of interface states based on the amphoteric model presented by Poindexter et al., which is a function of the assumed energy distribution when the tip rests near the junction and in different dc values, as the tip scans at two positions: $x=1.9$ μm and $x=3$ μm in the depletion and n-type neutral regions of the $p−n$ junction, respectively. The “spatial distribution” here is the net interface trapped charges density, $Q_{it}$, which is a function of the assumed energy distribution and the trap level occupancy Fermi function, calculated at discrete locations along the sample surface.

Secondly, the spatial distributions of the interface trapped charges around the SCM tip were calculated under the extracted dopant profile [see Fig. 1(a)] and different dc probe biases, $V_G$ ($V_G=−V_{dc}$), as the tip scans in two positions: $x=1.9$ μm and $x=3$ μm in the depletion and n-type neutral regions of the $p−n$ junction, respectively. The “spatial distribution” here is the net interface trapped charges density, $Q_{it}$, which is a function of the assumed energy distribution and the trap level occupancy Fermi function, calculated at discrete locations along the sample surface.

Thirdly, because interface states can not instantly respond to the UHF signal of the SCM sensor (915 MHz), and because the $V_{dc}$ applied to disturb the surface potential has been set as small as possible in the experiment (0.1 V), the interface trapped charges can be regarded as reacting only to $V_{dc}$. Thus, to account for the interface states’ behavior in SCM measurements, fixed charges subjected to the above spatial distributions, calculated at different $V_G$ values, were then, in turn, specified on the interface to replace the interface states in the simulation. A group of corresponding theoretical local C–V curves was then calculated over a range of $V_G$.

Finally, a theoretical $dC/dV$ value with respect to a certain $V_G$ value can be extracted from one of the local C–V curves, which corresponds to the spatial distribution of the charges obtained with that $V_G$ value, because, only at the point with respect to that $V_G$ value on this C–V curve, can both the simulated interface charges and the $V_G$ value match their experimental counterparts at the same time. The group of the obtained C–V curves can provide a group of local $dC/dV−V_G$ data to produce the final local $dC/dV−V_G$ plots. Doing this, the local $dC/dV−V_G$ characteristics obtained can be regarded as the theoretical counterpart of the experimental SCM output in the existence of interface states. The simulator used in the simulation is MEDICI software.

Figures 2(a) and 2(b) give the simulated spatial distributions of the interface trapped charges extracted under different $V_G$ values, as well as the dopant profiles near $x=1.9$ and $x=3$ μm. We can see from Fig. 2 that the maximum fringing area around the tip corresponding to the region where the $Q_{it}$ differs from that under the $V_G=0$ V condition is about 0.4 μm, and, within the fringing area, the spatial distribution of $Q_{it}$ changes significantly when the tip rests on different regions; that is, $Q_{it}$ is subjected to an asymmetric and symmetric distribution when the tip rests near the junction and in the neutral region, respectively. This is because only in the depletion region does there exit an energy band transition.
and the Fermi level become strongly position-sensitive. As a result, $Q_{\text{ii}}$ on the left side (the p-side) of the tip, as it scans near the junction, is always positive and, on the right side (the n-side) of the tip, is always negative due to the charging of the donor and acceptor interface states below and above the midgap, respectively [see Figs. 1(b) and 2(a)]. In practice, fixed charges subjected to the distributions were then placed on the interface in five segments within the fringing area (0.4 $\mu$m), with a mean value of the charges specified within each segment. This area of 0.4 $\mu$m can be proven to be wide enough by placing the charges within a wider region until no significant change can be seen in the simulated $C-V$ plots. The five segments can be proven, in the same way, to be dense enough for obtaining a consistent simulation result.

Figures 3(a) and 3(b) show the local $C-V$ and $dC/dV-V_G$ results at $x=1.9$ and $x=3.0$ $\mu$m extracted by the above mentioned method. Figure 3(a) shows that the local $C-V$ plots at $x=1.9$ $\mu$m are apparently stretched out, as well as shifted, by the interface states. This stretch-out is due to the fact that the absolute values of the voltages corresponding to the inversion and the accumulation conditions are increased, while the flatband voltages corresponding to the minimum capacitance in the $C-V$ plots have not been shifted to the same extent. As a result, both the positive and negative $dC/dV$ peaks at $x=1.9$ $\mu$m are depressed. Similar results were obtained at other positions near the junction in our simulation. However, compared with that at $x=1.9$ $\mu$m, the interface trapped charges cause a smaller parallel shift along the horizontal axis in the local $C-V$ curves at $x=3$ $\mu$m [Fig. 3(b)]. As a result, the $dC/dV-V_G$ curve at $x=3$ $\mu$m only becomes “fatter,” while the $dC/dV$ peak value remains almost unchanged. A similar result was obtained in the p-type neutral region in our simulation and can also be validated with other published experimental data.\textsuperscript{16} This effect of the interface states on the SCM $C-V$ characteristics can be attributed to the different spatial distributions of the trapped charges when the tip scans over the different regions of the p–n junction.

In summary, we have established a dedicated simulation model of interface states in the SCM measurement of p–n junctions. The simulation shows that the peak $dC/dV$ values decrease due to interface states only in the depletion region of the p–n junction, thus accounts for the discrepancy between the SCM experimental and simulation data near p–n junctions. Consequently, interface states are the crucial factor in SCM modeling and measurement, as well as dopant profiling of p–n junctions.

\begin{thebibliography}{9}
\bibitem{14}From the experimental $dC/dV-V_G$ data in Ref. 8, the transition from accumulation to inversion in the $C-V$ curves, which can be obtained by integrating $dC/dV$, is approximately 2 V, so that $V_{mn}=0.1$ V is small enough to keep the interface trapped charges nearly undisturbed.
\bibitem{15}\textsc{medet}: Two-Dimensional Device Simulation Program (TMA, Palo Alto, CA, 1997).
\end{thebibliography}