Published in the Journal of Vacuum Science and Technology,
vol. 11(3), May/June, 1993

Proceedings of the Topical Conference on Silicon-Based Heterostructures II

9–10 November 1992
Chicago Hyatt Regency
Chicago, Illinois

Supported by the
American Vacuum Society
and the
National Research Council, Canada

Proceedings Editor
Derek C. Houghton

Published for the American Vacuum Society by
the American Institute of Physics, New York 1993

Modeling of parasitic barrier effects in silicide/$Si_{1-x}Ge_x$ Schottky-barrier infrared detectors fabricated with a silicon sacrificial layer

X. Xiao, J. C. Sturm, S. R. Parihar, and S. A. Lyon
Princeton Photonics and Optoelectronics Materials Center (POEM), Department of Electrical Engineering, Princeton University, Princeton, New Jersey 08544

D. Meyerhofer, S. Palfrey, and F. V. Shallcross
David Sarnoff Research Center, Princeton, New Jersey 08543

(Received 15 October 1992; accepted 20 December 1992)

By employing a thin silicon sacrificial cap layer for silicide formation, we have fabricated both $Pd_2Si/Si_{1-x}Ge_x$ and $PtSi/Si_{1-x}Ge_x$ Schottky-barrier infrared detectors with extended cutoff wavelengths and near-ideal leakage characteristics. Substantial deviation in the spectral response from Fowler's theory was observed in some silicide/$Si_{1-x}Ge_x$ detectors fabricated using this technique. This deviation was attributed to a parasitic barrier at the interface due to the excess silicon sacrificial layer left unconsumed by the silicide formation process. A simple model which modifies Fowler's theory to take into account the reduced injection efficiencies of the photoexcited holes through the Si barrier was proposed. Good agreement between this model and the experimental data has been achieved.

I. INTRODUCTION

State-of-the-art silicide infrared focal-plane-array (FPA) technology is based on the PtSi/Si Schottky-barrier detector which has a cutoff wavelength of $\sim 5\ \mu m$. The PtSi/Si detector offers relatively high quantum efficiency and high uniformity, and it is compatible with standard complementary metal–oxide–semiconductor (CMOS) process technology.[1,2] For many applications, extending the cutoff wavelength of the silicide Schottky-barrier infrared detector into the 8–12 μm long-wavelength band would be advantageous. Strained $Si_{1-x}Ge_x$ on Si has a smaller band gap than silicon with most of the band offset in the valence band.[3,4] It is therefore expected from the Schottky–Mott model that a silicide/$Si_{1-x}Ge_x$ junction will have a smaller p-type Schottky-barrier height than will a silicide/Si junction, and therefore will have a longer cutoff wavelength.[5] The operation principle of the silicide/$Si_{1-x}Ge_x$ infrared detector, which was first proposed by Kanaya *et al.*,[5] is the same as that of a conventional silicide/Si Schottky-barrier detector (i.e., photoemission of holes from the silicide to the semiconductor). In the work of Kanaya *et al.*, no reverse bias electrical data or photoresponse was reported for a silicide/$Si_{1-x}Ge_x$ detector, however. Several later studies found that during the metal–$Si_{1-x}Ge_x$ reaction, palladium and platinum preferentially react with Si, causing Ge segregation.[6,7] This creates defects which pin the Fermi level[7] near midgap leading to a high Schottky-barrier height. In our work, by employing a thin silicon sacrificial layer for silicide formation on $Si_{1-x}Ge_x$, operation of $Pd_2Si/Si_{1-x}Ge_x$ and $PtSi/Si_{1-x}Ge_x$ Schottky-barrier long-wavelength infrared detectors has been demonstrated.[8,9] While the silicon sacrificial layer is required to prevent Fermi level pinning, excess silicon left unconsumed in the final device structure will adversely affect the spectral response of the detector. In this article, a model which takes into account the hole tunneling through the parasitic Si barrier has been proposed, and good agreement with the measured spectral response is demonstrated.

II. EXPERIMENTS AND RESULTS

Our samples were grown by rapid thermal chemical vapor deposition (CVD) on lightly doped p-type (100) substrates at 600–700 °C.[10] The structure consists of a fully strained $Si_{1-x}Ge_x$ alloy layer on top of a strained graded composition $Si_{1-y}Ge_y$ (y:0$\rightarrow x$) layer. The $Si_{1-x}Ge_x$ is capped by a thin sacrificial silicon layer which will be consumed later in silicide formation. The silicide was selectively formed inside deposited oxide windows using standard e-beam evaporation and annealing processes. We have fabricated both $Pd_2Si/Si_{1-x}Ge_x$ and $PtSi/Si_{1-x}Ge_x$ detectors. In the palladium devices, the targeted silicon sacrificial layer thickness was 100 Å, and the deposited palladium was nominally 150 Å. In the platinum devices, the sacrificial layer was 40 Å, and the metal was 25 Å. The Si cap and deposited metal thicknesses were chosen so that the silicon sacrificial cap layer would be exactly consumed in the silicide formation process. This process ensures a Schottky contact with a pure silicide film (without Ge) and, at the same time, eliminates the Ge segregation at the interface which could cause Fermi level pinning. Shown in Fig. 1 is a schematic cross section diagram of a fabricated silicide/$Si_{1-x}Ge_x$ detector. It should be noted that due to unavoidable variations in the silicon cap layer and deposited metal thicknesses, it is possible that a very thin layer of excess silicon was left in some devices or some $Si_{1-x}Ge_x$ was consumed.

Shown in Fig. 2 were the measured Fowler plots for three $Pd_2Si/Si_{1-x}Ge_x$ (x=0,0.20,0.35) and two $PtSi/Si_{1-x}Ge_x$ (x=0, 0.15) detectors at 77 K. It is clear that the cutoff wavelength increases with increasing Ge fraction for both Pd_2Si and PtSi detectors. The conventional Pd_2Si/Si Schottky diode has a barrier height of 420

 0734-211X/93/031168-04$01.00 ©1993 American Vacuum Society

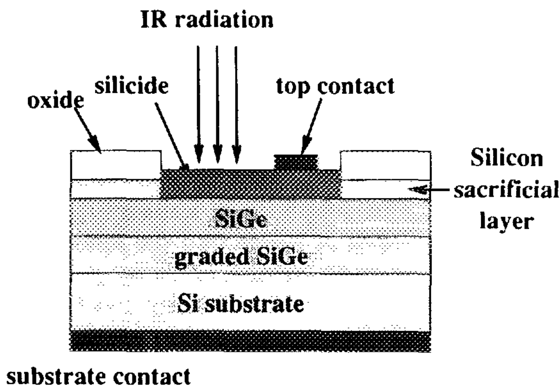
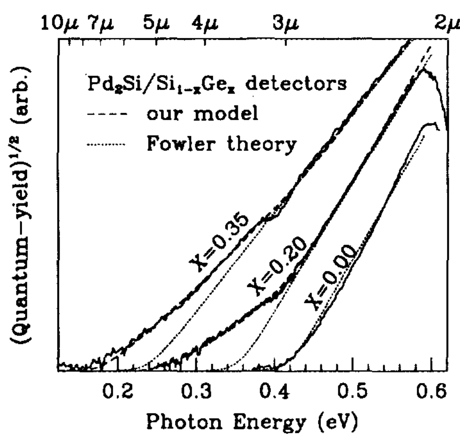


FIG. 1. Schematic cross section diagram of a silicide/$Si_{1-x}Ge_x$ Schottky-barrier infrared detector with a sacrificial silicon layer.

meV, which gives a cutoff wavelength of 3 μm. As Ge is introduced, the cutoff wavelengths of the $Pd_2Si/Si_{0.8}Ge_{0.2}$ and $Pd_2Si/Si_{0.65}Ge_{0.35}$ detectors have been pushed to about 5 and 7 μm, respectively. For the $PtSi/Si_{1-x}Ge_x$ detectors, the cutoff wavelength is extended from 5.2 to 8.8 μm with only 15% Ge in the alloy. It should be emphasized that a silicon sacrificial layer was required to achieve the desired barrier height reduction in the silicide/$Si_{1-x}Ge_x$ detectors. When the sacrificial layer was omitted, the barrier height of a $Pd_2Si/Si_{0.80}Ge_{0.20}$ detector (as measured by photoresponse) *increased* from 0.42 meV (for an all Si device) to 0.7 eV, indicating Fermi level pinning presumably due to Ge segregation during the silicide formation.[7]



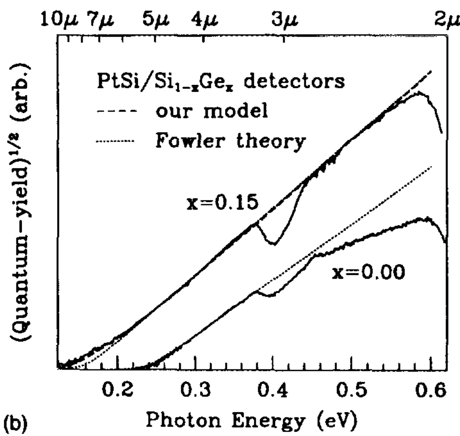


FIG. 2. Spectral response of (a) Pd_2Si and (b) PtSi Schottky-barrier infared detectors. The solid lines are experimental results measured by FTIR at 77 K. (The dip at 400 meV in some of these spectra is due to artifacts of the measurement instrument.) The dashed lines are best fits obtained using the parasitic barrier model developed in this work. The dotted lines are from Fowler's theory.

A more careful look at Fig. 2 reveals that not only do the silicide/$Si_{1-x}Ge_x$ detectors have reduced Schottky barrier heights compared to the pure silicon devices, but their spectral response curves also show a noticeable deviation from Fowler's theory. According to Fowler's theory, a plot of the square root of the quantum yield versus the photon energy for Schottky-barrier photoemission should be linear, as is observed for the Pd_2Si/Si device for photon energies above the barrier height by more than a few kT. This deviation is especially prominent for the $Pd_2Si/Si_{0.80}Ge_{0.20}$ detector. A kink is clearly visible in the Fowler plot around 400 meV, which matches very closely to the cutoff energy for the Pd_2Si/Si device. Even though much less pronounced, a similar kink exists around the same energy for the $Pd_2Si/Si_{0.65}Ge_{0.35}$ device as well. We attribute this change in the spectral response curve to a parasitic barrier in the valence band at the silicide/$Si_{1-x}Ge_x$ interface due to the excess of the silicon sacrificial layer which was left unconsumed in these devices (Fig. 3). This layer of excess silicon will result if the silicon sacrificial layer was thicker than designed or the deposited metal was thinner than expected due to imperfect thickness control. The $Pd_2Si/Si_{1-x}Ge_x$ devices were particularly susceptible to the parasitic barrier layer because of their initial thick (100 Å) silicon sacrificial layers. The width of the silicon barrier is expected to be very thin, however, most likely on the order of 1 nm or less. In order to gain a better understanding of the effect of this thin Si barrier on the spectral response of a silicide/$Si_{1-x}Ge_x$ detector, a modified Fowler theory has been developed.

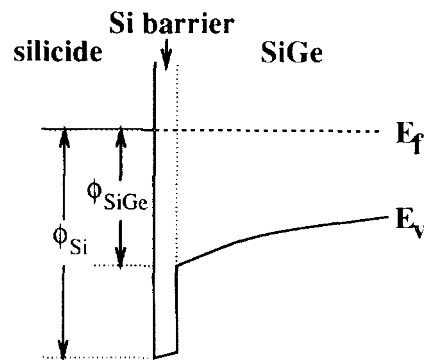


FIG. 3. Schematic band diagram of a silicide/$Si_{1-x}Ge_x$ detector with a parasitic silicon barrier.

III. THEORY

The process of photoemission at a metal/semiconductor interface involves the absorption of a photon by a free carrier inside the metal and subsequent injection of this photoexcited carrier from the metal into the semiconductor. It is so difficult to develop a complete and rigorous theoretical treatment that the most successful and most widely used theory today is still the general one which was developed by Fowler back in 1931.[11] At the heart of Fowler's theory lies the hypothesis that "the photoelectric sensitivity or number of electrons emitted per quantum of light absorbed is to a first approximation proportional to the number of electrons per unit volume of the metal whose kinetic energy normal to the surface augmented by $h\nu$ is sufficient to overcome the potential step at the surface." Based on this hypothesis, Fowler derived the following expression for the quantum yield[11]

$$Y \propto T^2 \int_0^\infty \ln(1+e^{-y+(h\nu-\phi_B)/kT})dy, \quad (1)$$

where $h\nu$ is the photon energy, ϕ_B is the barrier height, and T is the temperature. When the photon energy $h\nu$ is above the barrier height ϕ_B by more than a few kT, then the Fowler theory predicts $Y \propto (h\nu-\phi_B)^2$. If the square root of the quantum yield is plotted versus photon energy, it should give a straight line. By a simple linear extrapolation to zero quantum yield, an accurate value of barrier height can be obtained. The Fowler theory has been widely used to extract the barrier height from photoemission data in many different metal/semiconductor systems.

If excess sacrificial silicon is left unconsumed in our detector structure, an interfacial barrier due to the Si will face the holes as they attempt to reach the $Si_{1-x}Ge_x$. Figure 3 is a schematic band diagram of such a device. There are two barrier heights involved in this structure: the parasitic barrier height due to the thin Si layer (ϕ_{Si}) and the desired barrier height due to the underlying $Si_{1-x}Ge_x$ alloy (ϕ_{SiGe}). Because of the narrow width of the Si barrier, photoexcited holes will have a finite probability of tunneling though it even if their energy normal to the surface lies between ϕ_{Si} and ϕ_{SiGe}. Therefore, it is expected that this device would still have an apparent cutoff wavelength determined by ϕ_{SiGe}, just as a device without this barrier layer. The quantum yield will be reduced due to this barrier, however, especially when the photon energy lies between ϕ_{Si} and ϕ_{SiGe}. It is clear that the one parameter (the barrier height) Fowler theory cannot be directly applied in this situation.

To model the effects of this thin tunneling barrier on the spectral response curve, we propose a simple model based on following hypothesis which is very much in parallel to that of Fowler's theory: *the quantum yield is proportional to the integral of the hole-density of states in the metal weighted by their transmission coefficients through the silicon barrier into the* $Si_{1-x}Ge_x$ *layer, where the transmission coefficients are to be evaluated after the hole energies normal to the surface are augmented by the photon energy* $h\nu$.

One complication introduced in this model is the need to evaluate the transmission coefficient of a hole through the silicon barrier. A first principles calculation is extremely difficult because it would require not only detailed knowledge of the band structures of the metal, silicon, and strained $Si_{1-x}Ge_x$ alloy, but also knowledge of all wave functions involved. Therefore, in our model an approximation for calculating the hole transmission coefficient was used primarily for its simplicity of implementation. The transmission coefficient of a hole into the semiconductor was assumed to be zero for energies below ϕ_{SiGe}, a constant (T_0) for energies above ϕ_{Si}, and given by $T=T_0e^{-2\kappa w}$ for energies between ϕ_{Si} and ϕ_{SiGe}, where w is the Si barrier width, and κ is the imaginary part of the wave vector for a hole inside the barrier layer which was calculated using simple effective mass theory. Although simple, note that the model converges to Fowler's theory when the barrier width is zero (as in an ideal silicide/$Si_{1-x}Ge_x$ detector) or infinitely thick (as in a conventional silicide/Si device).

Based on the above hypothesis and assumption, it can be derived that the spectral response of a Schottky-barrier detector with a thin tunneling barrier is given by

$$Y(h\nu) \propto T^2 \Bigg[\int_0^\infty \ln(1+e^{-y+(h\nu-\phi_{Si})/kT})dy + \int_0^{(\phi_{Si}-\phi_{SiGe})/kT} \times \ln(1+e^{-y+(h\nu-\phi_{SiGe})/kT})e^{-A\sqrt{y}}dy \Bigg], \quad (2)$$

where $A = \sqrt{2m^*kTw^2/\hbar^2}$. The first term corresponds to photoemission of holes over the silicon barrier into the $Si_{1-x}Ge_x$ alloy, and it is identical to the results given by the Fowler theory for a barrier height of ϕ_{Si}. The second term, which vanishes at infinite barrier width w, represents the contribution from holes tunneling through the silicon barrier. When the barrier width w is zero, these two terms can be combined leading to a Fowler expression for a barrier height of ϕ_{SiGe}. The above equation was then numerically evaluated as a function of photon energy to obtain a spectral response.

IV. COMPARISON WITH DATA

Using the model developed above, we have calculated the spectral response of a $Pd_2Si/Si_{1-x}Ge_x$ detector with a parasitic silicon barrier, and the results for several different barrier widths are shown in Fig. 4. When the barrier layer is absent ($w=0$), the device is an ideal silicide/$Si_{1-x}Ge_x$ Schottky-barrier detector with a barrier height of 260 meV. The Fowler plot is a straight line, as expected from Fowler's theory. As the barrier width increases, the curve bends downward between ϕ_{SiGe} and ϕ_{Si} dragging down the yield for photoenergies above ϕ_{Si} as well. When the barrier width increases to 10 Å, a noticeable knee has developed around 420 meV. As the barrier width further increases to 50 Å, it essentially became a conventional pure silicon device without any barrier height reduction.

We have fit the experimental spectra shown in Fig. 2 with the model described above. The barrier height ϕ_{SiGe}, barrier width w, and a vertical scaling constant were three

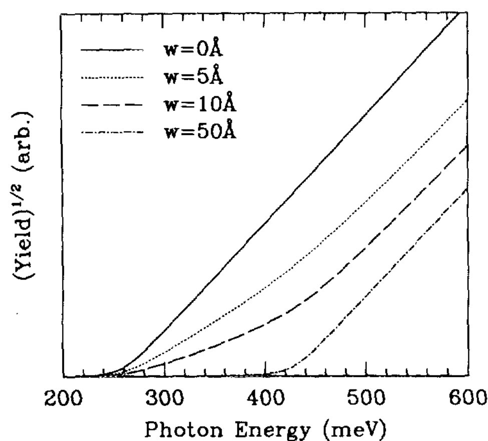


FIG. 4. Dependence of quantum yield on Si barrier width as calculated from Eq. (2) for a structure with the following parameters: $\phi_{Si}=420$ meV, $\phi_{SiGe}=260$ meV, $m^*=0.4\ m_0$, and $T=77$ K.

adjustable parameters. The values of ϕ_{Si} are obtained by fitting data of the pure Si devices to Fowler's theory. While ϕ_{SiGe} determines the apparent cutoff, the barrier width w determines the shape. Good agreement between our model and the experimental data has been achieved for all devices (Fig. 2). For example, while the Fowler theory gives a very poor fit to the $Pd_2Si/Si_{0.80}Ge_{0.20}$ detector, an excellent agreement was obtained with our parasitic barrier model using a barrier width of 10 Å. This excess Si could have resulted from a Si cap deposited in excess of the desired 100 by 10 Å, or from an evaporated Pd 15 Å thinner than expected. It was thought that the evaporated Pd reacted to completion during a 10 min anneal at 200 °C. Similarly, for the $Pd_2Si/Si_{0.65}Ge_{0.35}$ device, a best fit yielded a barrier width of 3 Å. Such errors in thickness are reasonable given the repeatability in our laboratory.

For the $PtSi/Si_{0.85}Ge_{0.15}$ device, however, fitting the data with our model gives only minor improvement over that obtained with the Fowler theory, indicating a very thin Si barrier. A best fit was obtained with an interfacial Si barrier width of ~3 Å. This is consistent with the fact that a much thinner Si sacrificial layer was used in the $PtSi/Si_{1-x}Ge_x$ device compared to that in the $Pd_2Si/Si_{1-x}Ge_x$ devices (40 vs 100 Å). Therefore the PtSi device was much less susceptible to the adverse effect of an interface Si barrier than the Pd_2Si detectors.

V. SUMMARY

In summary, by using a silicon sacrificial cap layer for silicide formation, we have demonstrated $Pd_2Si/Si_{1-x}Ge_x$ and $PtSi/Si_{1-x}Ge_x$ Schottky-barrier infrared detectors with extended cutoff wavelengths. While a direct metal–$Si_{1-x}Ge_x$ reaction would result in an increased barrier height presumably due to Ge segregation and consequent Fermi level pinning, an excess of the Si sacrificial layer left unreacted would function as an undesired parasitic barrier which adversely affects the quantum efficiency of the detector. A simple model has been developed for the effect of this parasitic barrier on the spectral response of a silicide/$Si_{1-x}Ge_x$ detector. It is found that a very tight control of the silicon sacrificial layer thickness (on the order of 1 nm) is required to achieve high performance in these type of detectors.

ACKNOWLEDGMENTS

This work is supported by the New Jersey Commission on Science and Technology, the National Science Foundation, and the Office of Naval Research.

[1]W. F. Kosonocky, Proc. SPIE **1308**, 2 (1990).
[2]D. J. Sauer, F. L. Hsueh, F. V. Shallcross, G. M. Meray, and T. S. Villani, Proc. SPIE **1308**, 81 (1990).
[3]C. G. Van de Walle and R. M. Martin, Phys. Rev. B **34**, 5621 (1986).
[4]R. People and J. C. Bean, Appl. Phys. Lett. **48**, 538 (1986).
[5]H. Kanaya, F. Hasegawa, E. Yamaka, T. Moriyama, and M. Nakajima, Jpn. J. Appl. Phys. **28**, L544 (1989).
[6]H. Kanaya, Y. Cho, F. Hasegawa, and E. Yamaka, Jpn. J. Appl. Phys. **29**, L850 (1991).
[7]H. K. Liou, X. Wu, U. Gennser, V. P. Kesan, S. S. Iyer, K. N. Tu, and E. S. Yang, Appl. Phys. Lett. **60**, 577 (1992).
[8]X. Xiao, J. C. Sturm, S. R. Parihar, S. A. Lyon, D. Meyerhofer, and S. Palfrey, IEDM Tech. Dig. (to be published).
[9]X. Xiao, J. C. Sturm, S. R. Parihar, S. A. Lyon, D. Meyerhofer, and S. Palfrey (unpublished).
[10]J. C. Sturm, P. V. Schwartz, E. J. Prinz, and H. Manoharan, J. Vac. Sci. Technol. B **9**, 2011 (1991).
[11]R. H. Fowler, Phys. Rev. **38**, 45 (1931).