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13. ABSTRACT (Maximum 200 words)

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This project utilized a variety of experimental methods to produce thin films of SiGeC on Si for the purpose of creating a heteroepitaxial layer with a different energy bandgap on the substrate Si for applications to bipolar transistors. Growth was performed by combined ion and molecular beam deposition, by CVD and by C ion implantation. Up to 3 atomic percent C was successfully incorporated. Theoretical and experimental bandgaps decreased with increasing C content for up to 1.5 percent C.

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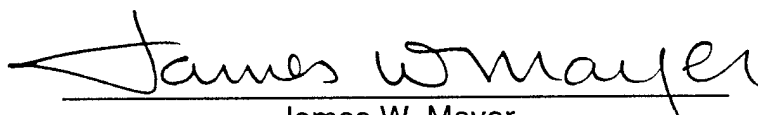
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James W. Mayer
Principal Investigator

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Final Technical Report

Heteroepitaxy of Ternary SiGeC Alloys on Si for Bipolar Transistors

Summary

- i) Technical problem: Form and characterize layers of SiGeC on Si for the purpose of creating a heteroepitaxial layer with a different energy bandgap on the substrate Si for applications to bipolar transistors.
- ii) General methodology is to utilize a variety of experimental methods to grow the films and to use ion, electron and photon technologies to characterize the films. There is a theoretical effort to predict the energy band structure.
- iii) Technical results:
 - a) Growth of SiGeC on Si, SiGeC layers were formed by ion implantation of C into SiGe (Cornell University and Arizona State University), by Chemical Vapor Deposition (CVD) (Lawrence Semiconductor Research Laboratory and Arizona State University) and by Combined Ion and Molecular Beam Deposition at Arizona State University. The key finding was that up to 2 atomic percent carbon could be incorporated to form high-quality heteroepitaxial layers of SiGeC on 100 Si. Under proper CVD growth conditions up to 3 atomic percent could be incorporated; higher carbon concentrations resulted in defected or amorphous layers.
 - b) Analysis. The layers were evaluated by a number of analytical techniques at Arizona State University. MeV He ion beam analysis by backscattering and channeling, secondary ion mass spectrometry, x-ray diffraction, raman spectroscopy, atomic force microscopy, transmission electron microscopy, and electrical characterization. The key results were that carbon could be incorporated on substitutional lattice sites to C concentrations up to 2 atomic percent with strain compensation and layer thicknesses in excess of the heteroepitaxial limit for SiGe on (100) Si.
 - c) Theory and Bandgap Experimental results for carbon concentrations up to 1.5 atomic percent indicate the energy band gap decreases with increased C and Ge concentrations as predicted by theory.
 - d) Principal collaborators: R. Soref of AF Rome Laboratories for fabrication of waveguides and Prof. J. Kolodzey of the University of Delaware.
 - e) Theses and Publications. The following pages list 50 journal publications, 13 PhD theses and 3 M.S. theses that acknowledge ARPA/AFOSR support.
- iv) Implications for Further Research:

This program showed that high quality SiGeC layers could be grown heteroepitaxially on 100 Si. A broader based program was funded by DARPA for a "Consortium on Silicon Nanoelectronics (COSIN)", DARPA Nanoelectronics Program Agreement No. MDA972-95-3-0047, on Silicon-based Nanostructures for Ultra-high Performance Silicon Circuits". The Consortium involves Hughes Research Laboratories, Lawrence Semiconductor Research Laboratories, Arizona State University, Auburn University, Stanford University and University of California at San Diego.

ASU Publications on SiGeC (AFOSR/ARPA support acknowledged)

1. Metastable SiGeC formation by solid phase epitaxy
J.W. Strane, H.J. Stein, S.R. Lee, B.L. Doyle, S.T. Picraux and J.W. Mayer
Appl. Phys. Lett. 63, 2786 (1993)
2. Precipitation and relaxation in strained Si_{1-y}C_y/Si heterostructures
J.W. Strane, H.J. Stein, S.R. Lee, S.T. Picraux, J.K. Watanabe and J.W. Mayer
J. Appl. Phys. 76, 3656 (1994)
3. Chemical vapor deposition of heteroepitaxial Si_{1-y}Ge_xC_y films on (100)Si substrates
Z. Atzmon, A.E. Bair, E.J. Jaquez, J.W. Mayer, D. Chandrasekhar, D.J. Smith and R.L. Hervig
Appl. Phys. Lett. 65, 2559 (1994)
4. Novel chemical routes to silicon-germanium-carbon materials
J. Kouvetakis, M. Todd, D. Chandrasekhar and D.J. Smith
Appl. Phys. Lett. 65, 2960 (1994)
5. Raman spectroscopy study of microscopic strain in epitaxial Si_{1-y}Ge_xC_y alloys
J. Menéndez, P. Gopalan, G.S. Spencer, N. Cave and J.W. Strane
Appl. Phys. Lett. 66, 1160 (1995)
6. Theoretical investigation of random Si-C alloys
A.A. Demkov and O.F. Sankey
Phys. Rev. B48, 2207 (1993)
7. Carbon Incorporation into Si at High Concentrations by Ion Implantation and Solid Phase Epitaxy
J.W. Strane, S.R. Lee, H.J. Stein, S.T. Picraux, J.K. Watanabe and J.W. Mayer
J. Appl. Phys. 79 (2), 637-646 (1996)
8. Wet Oxidation of Amorphous and Crystalline Si_{1-x-y}Ge_xC_y Alloys Grown on (100)Si Substrates
Z. Atzmon, A.E. Bair, T.L. Alford, J.W. Mayer, D. Chandrasekhar and David J. Smith
Appl. Phys. Lett. Vol. 66 (17), pp. 2244-2246 (1995)
9. Quantification of carbon in Si_{1-x-y}Ge_xC_y with uniform profiles.
A.E. Bair, Z. Atzmon, S.W. Russell, T.L. Alford, J.W. Mayer and J.C. Barbour
Nuclear Instruments and Methods in Physics Research B103, 339-346 (1995)
10. Epitaxial Growth and Characterization of Ge_{1-x}C_x Alloys on Si(100)
M. Krishnamurthy, Jeff Drucker and A. Challa
J. Appl. Phys. 78 (2), 7070-7073 (1995)
11. Growth of heteroepitaxial Si_{1-x-y}Ge_xC_y alloys on silicon using novel deposition chemistry
M. Todd, P. Matsunaga, J. Kouvetakis, D. Chandrasekhar and D.J. Smith
Appl. Phys. Lett. 67, 1247 (1995)
12. TEM characterization of SiGeC material system
D. Chandrasekhar, D.J. Smith, J. Kouvetakis and McD. Robinson
Proc. 53rd Ann. Meet. MSA (San Francisco Press, San Francisco, 1994) pp. 840-841

13. The onset of secondary phase precipitation during synthesis of heteroepitaxial $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ on Si(100)
N. Herbots, P. Ye, H. Jacobsson, J. Xiang, S. Hearne and N. Cave
Appl. Phys. Lett. 68, 782 (1996)
14. Comparative study on dry oxidation of heteroepitaxial $\text{Si}_{1-x-y}\text{Ge}_x$ and $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ on Si(100)
J. Xiang, N. Herbots, H. Jacobsson, P. Ye, S. Hearne and S. Whaley
J. Appl. Phys. 80 (3), (1 Aug 1996)
15. Characterization of carbon in heteroepitaxial $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ thin films via combined ion channeling and nuclear resonance analysis
S. Hearne, N. Herbots, J. Xiang, P. Ye and H. Jacobsson
Nucl. Instrum. Methods B (accepted)
16. Microstructure and ion beam characterization of heteroepitaxial $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$
H. Jacobsson, P. Ye, N. Herbots, S. Hearne and J. Xiang
Nucl. Instrum. Methods B, accepted (1995)
17. Measuring the tensor nature of stress in silicon using polarized off-axis Raman spectroscopy
G.H. Loechelt, N.G. Cave and J. Menéndez
Appl. Phys. Lett. 66, 3639 (1995)
18. Energy band gaps of silicon-carbon alloys
J. Gryko and O.F. Sankey
Phys. Rev. 1351, 7295 (1995)
19. Heteroepitaxial $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ Films on (100)Si Substrates for Future Low-Power Applications
T.L. Alford, A.E. Bair, Z. Atzmon, L.M. Stout, S.G. Balster, D.K. Schroder and R.J. Roedel
Thin Solid Films (accepted)
20. Mechanisms and kinetics of wet oxidation of amorphous $\text{Si}_{1-y}\text{Ge}_x\text{C}_y$ grown on (100)Si substrates
A.E. Bair, Z. Atzmon, T.L. Alford and D.J. Smith
J. Appl. Phys. (submitted)
21. An x-ray diffraction study of the strain and structure of SiGeC/(100)Si alloys
A.E. Bair, T.L. Alford, S. Segó, Z. Atzmon and R.J. Culbertson
Materials Chemistry and Physics (accepted)
22. The effect of carbon on Ti metallization and strain relaxation of Ti/ $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ thin films epitaxially grown on Si (001)
A. Eyal, R. Brener, R. Beserman, M. Eizenberg, Z. Atzmon, D.J. Smith and J.W. Mayer
Appl. Phys. Lett. 69 (1), 64 (1 July 1996)
23. Strain measurement of SiGeC heteroepitaxial layers on Si(001) using ion beam analysis
S. Segó, R.J. Culbertson, D.J. Smith, Z. Atzmon and A.E. Bair
J. Vac. Sci. Tech., in press (1996)

24. Defect and strain analysis of $\text{Si}_{1-y}\text{Ge}_x\text{C}_y$ films grown epitaxially on (100)Si via RBS and TEM
Z. Atzmon, A.E. Bair, S. Segó, D.J. Smith, D. Chandrasekhar and J.W. Mayer
Nucl. Inst. Methods, in press (1996)
25. Growth and characterization of heteroepitaxial $\text{Si}_{1-y}\text{Ge}_x\text{C}_y$ alloys
D.J. Smith, A. Amali, D. Chandrasekhar, Z. Atzmon, A.E. Bair, McD. Robinson and R. Westhoff
J. Appl. Phys., accepted (1996)
26. On the heteroepitaxial properties of $\text{Si}_{1-y}\text{Ge}_x\text{C}_y$ on Si(100) grown by combined ion and molecular beam deposition
H. Jacobsson, J. Xiang, N. Herbots, S. Whaley, P. Ye and S. Hearne
J. Appl. Phys., accepted (1996)

Materials Research Society Symposia Proceedings

27. Stability and precipitation kinetics in $\text{Si}_{1-y}\text{C}_y/\text{Si}$ and $\text{Si}_{1-y}\text{Ge}_x\text{C}_y/\text{Si}$ heterostructures prepared by solid phase epitaxy
J.W. Strane, S.T. Picraux, H.J. Stein, S.R. Lee, J. Candelaria, D. Theodore and J.W. Mayer
Fall 1993 Boston
28. Influence of precursor chemistry on synthesis of silicon-carbon-germanium alloys
M. Todd, J. Kouvetakis, P. Matsunaga, D. Chandrasekhar and D.J. Smith
Mat. Res. Soc. Symp. Proc., in press.
29. Heteroepitaxial $\text{Si}_{1-y}\text{Ge}_x\text{C}_y$ layer growth on (100)Si by atmospheric pressure chemical vapor deposition
Z. Atzmon, A.E. Bair, T.L. Alford, D. Chandrasekhar, D.J. Smith and J.W. Mayer
30. Wet oxidation of $\text{Si}_{1-y}\text{Ge}_x\text{C}_y$ layers on (100)Si
A.E. Bair, Z. Atzmon, T.L. Alford, D. Chandrasekhar and D.J. Smith
31. Characterization by Nuclear Resonance Combined with Ion Channeling of Heteroepitaxial $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ synthesized by CIMD on Si(100)
S. Hearne, N. Herbots, P. Ye, J. Xiang and H. Jacobsson
1994 Fall Meeting, Nov. 27-Dec. 2, Boston, MA
32. Ion implantation of SiGeC heteroepitaxial layers on Si(100) substrates with Ar^+ ions
Roger Garcia, Kurt E. Daley, Robert J. Culbertson, Nicole Herbots and Peihua Ye
1994 Fall Meeting, Nov. 27-Dec. 2, Boston, MA
33. Strain measurements of SiGeC heteroepitaxial layers on Si(100) using ion beam analysis
S. Segó, T. Alford, Z. Atzmon, A.E. Bair, K. Daley, P. Ye, S.H. Shiu, R.J. Culbertson and N. Herbots
1994 Fall Meeting, Nov. 27-Dec. 2, Boston, MA
34. Thermal oxidation of heteroepitaxial $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ alloy thin films
N. Herbots, P. Ye, S. Hearne and H. Jacobsson
1994 Fall Meeting, Nov. 27-Dec. 2, Boston, MA

35. Synthesis of heteroepitaxial $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y/\text{Si}(100)$ by combined ion and molecular beam deposition (CIMD): the role of temperature
N. Herbots, Peihua Ye, Jiong Xiang, Sean Hearne and Harald Jacobsson
1994 Fall Meeting, Nov. 27-Dec. 2, Boston, MA
36. Wet chemical cleaning of $\text{Si}(100)$ surfaces - ion beam characterization using elastic recoil and nuclear resonance techniques
V. Atluri, N. Herbots, S. Whaley, S. Bhagvat, P. Ye and R. J. Culbertson
1994 Fall Meeting, Nov. 27-Dec. 2, Boston, MA
37. An AFM study of $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ alloy thin films ($0.3 \leq x \leq 0.5$ and $0 \leq y \leq 0.1$) as a function of epitaxial quality and carbon content
S. Whaley, N. Herbots, J. Xiang, P. Ye, H. Jacobsson, S. Hearne, S. Segó and R.J. Culbertson
Spring Meeting, San Francisco, April 17-21 1995
38. Correlation between the dry oxidation rates and the strain in epitaxial $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ alloy thin films
J. Xiang, S. Segó, P. Ye, S. Hearne, H. Jacobsson, S. Whaley, N. Herbots and R. J. Culbertson
Spring Meeting, San Francisco, April 1995
39. Characterization of Sb-implanted SiGeC heteroepitaxial layers on $\text{Si}(001)$
R. Garcia, K.E. Daley, S. Segó, R.J. Culbertson and D.B. Poker
Spring Meeting, San Francisco, April 1995
40. Growth Morphology of Ag Islands on GaAs (110) at Low Coverage: Monte Carlo Simulations
A. Challa, T.S. Cale and J. Drucker
1994 Fall Meeting, Nov. 27-Dec. 2, Boston, MA

American Vacuum Society, Proceedings

41. Ion beam characterization of $\text{Si}(100)$ surfaces during wet chemical cleaning
V. Atluri, N. Herbots, P. Ye and R.J. Culbertson
Annual Meeting, Denver, October 24-28, 1994
42. Strain measurements of SiGeC heteroepitaxial layers on $\text{Si}(100)$ using ion beam analysis
S. Segó, A. Bair, K. Daley, P. Ye, R.J. Culbertson and N. Herbots
Annual Meeting, Denver, October 24-28, 1994
43. Sb ion implantation and annealing of SiGeC heteroepitaxial layers on $\text{Si}(001)$
R. Garcia, T. Alford, K. Daley, S. Segó, S.H. Shiu, R.J. Culbertson and D.B. Poker
Annual Meeting, Denver, October 24-28, 1994

International Conference on Ion Beam Analysis, Tempe, AZ, May 1995
Nucl. Instr. Meth. (submitted)

44. Ion beam analysis of heteroepitaxial SiGeC films on (100)Si substrates
Z. Atzmon, A.E. Bair, J.W. Mayer, D. Chandrasekhar and D.J. Smith
Invited Presentation
45. Microstructure and ion beam characterization of epitaxial $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ films
Harald Jacobsson, Peihua Ye, Nicole Herbots, Joan Xiang and Sean Hearne
46. Effect of carbon on dry oxidation of heteroepitaxial $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ alloy thin films
J. Xiang, N. Herbots, P. Ye, H. Jacobsson, S. Hearne and S. Segó
47. Hydrogen passivation of Si(100) wafers as templates for low temperature eptiaxy:
characterization by combined nuclear resonance analysis/ion channeling and H-recoil
V. Atluri, N. Herbots, S. Bhagvat and S. Whaley
48. Carbon nuclear resonance analysis combined with $\langle 110 \rangle$ and $\langle 111 \rangle$ ion channeling of
heteroepitaxial $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$: discrimination between surface and thin film carbon
S. Hearne, N. Herbots, H. Jacobsson, J. Xiang and P. Ye
49. Ion beam induced epitaxial crystallization of $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$
S. Segó, K. Daley, R. Garcia, R.J. Culbertson and N. Herbots
50. Comparison of elastic resonance and elastic recoil detection in the quantification of
carbon in SiGeC
A.E. Bair, Z. Atzmon, S.W. Russell, J.C. Barbour, T.L. Alford and J.W. Mayer

Ph.D. Theses

1. *Formation and Thermal Stability of SiGeC Alloys made by Ion Implantation and Solid Phase Epitaxy*
J.W. Strane, May 1994
2. *Electronic Structure Approach to Complex Systems*
Alexander A. Demkov, June 1995
3. *Synthesis and Characterization of Heteroepitaxial $Si_{1-x-y}Ge_xC_y$ Alloys on Si(100)*
Peihua Ye, August 1995
4. *Characterization, Oxidation and Metallization of SiGeC Alloys Grown by Chemical Vapor Deposition*
Andrew E. Bair, April 1996
5. *Microstructure Evolution During the Early Stages of Deposition*
Ashok Challa, February 1996
6. *Strain in SiGeC Thin Films*
Sean Segó, May 1996
7. *Ion Beam Modification and Characterization of SiGeC Thin Films*
Roger Garcia, February 1996
8. *Dry and Rapid Thermal Oxidation of SiGeC Thin Films*
Joan Xiang, June 1996
9. *Chemical Vapor Deposition of SiGeC Solid Solutions*
Pankaj Joshi, June 1996
10. *Device Fabrication and Material Characterization in $Si_{1-x-y}Ge_xC_y$*
Larry Stout, August 1996
11. *Surface Morphology of SiGe and SiGeC Films*
Ying Hong, August 1996
12. *SiGeC Heterojunction Bipolar Transistors, Vertical PN Junctions and Dopant Incorporation*
Scott Balster, December 1996
13. *Growth and Characterization of SiC and SiGeC Heteroepitaxial Alloys*
Durvasulu Chandrasekhar, March 1997

Master Theses

1. *Raman Spectroscopy of Silicon-Germanium-Carbon Alloys*
P.S. Gopalan, December 1994
2. *Quantitative Analysis of AFM Topographs of Si(100), SiGe(100) and SiGeC Surfaces*
Sean Whaley, December 1995
3. *Oxidation of SiGeC Thin Films*
John Theisen, May/August 1996