Wednesday Afternoon, October 4, 2000

Semiconductors
Room 306 - Session SC+EL+SS-WeA
Semiconductor Alloys

Moderator: P. Desjardins, Ecole Polytechnique de Montreal

2:00pm **SC+EL+SS-WeA1 Si-Ge Heterostructures***, **K.L. Wang**,* University of California, Los Angeles **INVITED**

PLEASE SEND US AN ABSTRACT. Thank you.

2:40pm **SC+EL+SS-WeA3 Critical Behavior of Epitaxial Si@sub 1-x@Ge@sub x@/Si(001) Islands***, **R.A. Budiman**, H.E. Ruda, D.D. Perovic, B. Bahierathan,* University of Toronto, Canada

We study the island size distributions of three-dimensional Si@sub 1-x@Ge@sub x@/Si(001) islands of varying Ge fractions (x = 0.4-0.7) and thicknesses grown by ultrahigh vacuum chemical vapor deposition. The size distributions of the percolating islands obey the dynamic scaling hypothesis due to random percolation process, only in the small island limit. Morphologies of the islands strongly suggest a presence of Smoluchowski ripening mechanism, in which islands collide and ripen. We therefore combine random percolation and Smoluchowski ripening to analyze the size distributions. To understand the critical behavior of the islands as exhibited by their size distributions, we formulate a mean-field theory of coherently strained island formation by incorporating surface energy and strain relaxation. The resulting phase diagram shows that the island formation in Si@sub 1-x@Ge@sub x@/Si(001) is located near the critical region. Order parameter fluctuations can be estimated by calculating the curvature energy for such a system and we find that the strain fluctuation is indeed relevant to properly describe the island formation in the Si@sub 1-x@Ge@sub x@/Si(001) system.

3:00pm **SC+EL+SS-WeA4 Growth of Coherent Three-dimensional Si Islands on Ge(111)***, **A. Raviswaran**, C.P. Liu,* University of Illinois, Urbana-Champaign*; J.M. Gibson,* Argonne National Laboratory*; D.G. Cahill,* University of Illinois, Urbana-Champaign

We study the evolution of three-dimensional islands during Si/Ge(111) epitaxy. The strain due to lattice mismatch (4.2% tensile) and the difference in the surface energies (@gamma@@sub Si@>@gamma@@sub Ge@) contribute to the formation of the three-dimensional Si islands. We grow Si islands on pseudomorphic Si@sub 0.15@Ge@sub 0.85@ buffer layers (deposited on Ge(111) substrates) in the temperature range 500°C - 650°C using MBE; the (111) orientation is used because the critical thickness of Si layers on Ge(111) is larger than that on Ge(001). We characterize the morphology and relaxation of the Si islands using ex situ AFM, TEM and SEM. Islanding occurs at 1 BL Si coverage, i.e., without the formation of a wetting layer. We observe high densities (~ 10@super 12@ cm@super -2@) of coherent, circular base islands for growth temperatures 500°C - 600°C and low Si coverage (< 2 BL Si). The density and shape of the islands is insensitive to the growth temperature. Beyond a critical width the islands relax plastically, by the nucleation and glide of misfit dislocations; this critical width is ~ 16 nm at 550°C and ~ 25 nm at 600°C. We observe large, incoherent, irregularly shaped islands at higher temperatures (> 600°C) and coverages (> 4 BL Si). As the islands transform from coherent to incoherent, coarsening occurs which results in an increase in the island width and a reduction in the island density. The high temperature (> 600°C) growths show a secondary maximum in the island density near 4 BL Si coverage.

3:20pm **SC+EL+SS-WeA5 Adatom Assisted Stabilization of Ad-dimers on Ge(001)***, **E. Zoethout**, H.J.W. Zandvliet, B. Poelsema,* University of Twente, The Netherlands

Studies of the early stage of near room temperature growth of silicon on Ge(001) have revealed an inconsistency between experimental@footnote 1@ and theoretical@footnote 2@ work. Experimentally a stable cluster has been labeled to be a trough dimer oriented perpendicular to the substrate dimer bonds (D-dimer). The same type of cluster is found in the early stage of near room temperature homoepitaxial growth on Ge(001). Theoretically such a D-dimer is predicted to be energetically unfavorable. It turns out that the apparent D-dimer is actually comprised of three rather than two atoms. The three-atom cluster of Ge or Si on Ge(001) is shown to differ from a trough dimer orientated along the substrate dimer bonds, from a small epitaxial island and also from a three-atom Si cluster on Si(001). The three-atom cluster of Ge or Si on Ge(001) is composed of an ad-dimer in the D-configuration and an adatom on the neighboring substrate dimer row. @FootnoteText@ @Footnote 1@W. Wulfhekel, B.J. Hattink, H.J.W. Zandvliet, G. Rosenfeld, and B. Poelsema, Phys. Rev. Lett. 79, 2494 (1997). @Footnote 2@S.V. Khare, R.V. Kulkarni, D. Stroud and J.W. Wilkins, Phys. Rev. Lett. 60, 4458 (1999).

3:40pm **SC+EL+SS-WeA6 C Incorporation during the Growth Of Ge@sub 1-y@C@sub y@/Ge(001) from Hyperthermal Beams***, **J. D'Arcy-Gall**, D. Gall, P. Desjardins, I. Petrov, J.E. Greene,* University of Illinois, Urbana

C-containing group-IV semiconductor alloys are of interest due to the potential they offer for both band gap and strain engineering in microelectronics. This investigation focuses on the effects of incident particle energy and film growth temperature T@sub s@ on the distribution of C lattice configurations in Ge@sub 1-y@C@sub y@ epitaxial layers grown on Ge(001) from hyperthermal beams obtained by ultra-high vacuum ion-beam sputtering using Kr@super +@. All Ge@sub 1-y@C@sub y@ (y @<=@ 0.03) layers, grown at T@sub s@ = 245-415 °C, are fully-coherent and free of extended defects as judged by high-resolution x-ray diffraction, reciprocal lattice mapping, and transmission electron microscopy. The strain-state of epitaxial Ge@sub 0.99@C@sub 0.01@ alloys grown at T@sub s@ = 300 °C changes from in-plane tension to compression as the Kr@super +@ energy E@sub Kr@ is increased from 300 to 900 eV. This results from an increasing fraction of C incorporated in Ge-C split interstitial sites as a result of the trapping, by substitutional C, of Ge self-interstitials formed due to irradiation by the increasing fraction of sputtered Ge atoms in the high energy tail of the energy distribution. These results are supported by TRIM simulations which show that the number of displaced lattice atoms per incident hyperthermal Ge increases from 0.10 with E@sub Kr@ = 300 eV to 0.24 at 900 eV, and ab initio calculations of layer strain for different C lattice configurations. All Ge@sub 1-y@C@sub y@ alloys grown at E@sub Kr@ = 900 eV are in a state of in-plane compression, which decreases with increasing T@sub s@. Raman scattering results show that the substitutional C concentration in these layers is negligible. Comparison of experimental results with ab initio calculations reveals that an increasing fraction of C incorporates as C pairs as T@sub s@ is increased due to the higher C-C encounter probability on the growth surface.

4:00pm **SC+EL+SS-WeA7 Growth and Characterization of Metastable Ge@sub1-x@C@subx@ Thin Films on Si(100) Substrate.***, **W. Li**, D. Guerin, S.I. Shah,* University of Delaware

The Ge-C system is of interest due to the possibility of band gap engineering on Si. For strain free deposition of Ge@sub1-x@C@subx@, a carbon concentration in excess of 10% is required, assuming that the system obeys Vegard's law. The maximum equilibrium solubility of C in Ge, however, is only 10@super8@/cm@super3@. Molecular beam epitaxy and chemical vapor deposition have been used to grow metastable Ge@sub1-x@C@subx@ thin films with x up to 2.5%. We have used a bias assisted sputter deposition using Ge and C magnetrons to obtain the epitaxial Ge@sub1-x@C@subx@ films with extended carbon solubility. Without any applied substrate bias and C flux, a Ge epitaxial layer on Si(100) substrate was obtained at 750°C with proper substrate preparation. Based on the results of pure Ge epitaxy, C was systematically added. Without the substrate bias, x-ray diffraction analyses show that the films were polycrystalline. With the application of a substrate bias, we were able to obtain epitaxial Ge@sub1-x@C@subx@ films. The Ge (400) XRD peak shifts to higher 2@theta@ were observed indicating C incorporation in the Ge lattice. Extended x-ray absorption fine structure (EXAFS) analyses confirmed that the C was indeed incorporated on the substitutional sites in the Ge lattice. C concentration was determined from XRD, X-ray photoelectron spectroscopy (XPS) and Rutherford backscattering spectroscopy (RBS). A C concentration of up to 5 at.% was obtained. Depth profiles of samples by XPS show that carbon is uniformly distributed in the film. Experiments are underway to study the effects of bias and thickness on the epitaxial deposition of Ge@sub1-x@C@subx@ with even further extension of the concentration of substitutionally situated C in germanium lattice.

4:20pm **SC+EL+SS-WeA8 Electrical and Optical Properties of Silicon : Germanium Alloys prepared by DC Magnetron Sputtering***, **A. Subrahmanyam**, S. Karthikeyan, J. Asbalter,* Indian Institute of Technology, Madras, India*; P. Amirtharaj,* National Institute of Standards and Technology

The Silicon: Germanium (Si:Ge) alloys are being used in various semiconductor devices. As is well known, these alloys offer advantages in band gap engineering, and can integrate well with the existing silicon technology. Several studies have been made on these alloys. In the present paper, we report the electrical and optical properties of Si:Ge alloys prepared by DC Magnetron sputtering technique. A 7.5 cm diameter circular magnetron cathode has been designed and fabricated. The balanced magnetron cathode is operated at low pressures (4.0 x 10@super -3@ mbar). Argon is the sputter gas. The target is prepared by bonding commercially available Silicon wafer to the water cooled copper backing plate. A small portion of the erosion area on the magnetron cathode is covered with pure germanium wafer. The alloys of Si:Ge (undoped) are prepared (at room temperature 25°C) on glass and Si substrates. The growth parameters in the present study are : flow rate of argon (180 - 250 sccm), Magnetron power (80 - 225 watts) and germanium content in the alloy. The thickness and refractive index of the films is measured by ellipsometer in the wavelength range 300 - 700 nm. The thickness of these alloy films is about 150 nm. The alloy films have been found to be amorphous. The germanium content in the alloy films is varied between 15 - 30 atomic % and is estimated by EDAX and RBS analysis. The optical absorption and photo conductivity measurements have been made on these alloys. The optical band gap of these alloys is in the range 1.45 - 1.6 eV. The dark conductivity is in the order 10@super-@ mho cm@super-1@. The deposition rate is observed to be linear with the magnetron power till 120 watts.

4:40pm **SC+EL+SS-WeA9 Preparation and Characterization of Highly Li-doped a-Se Alloy Films for Thermal Neutron Detectors***, **K.C. Mandal**, B. Dille, R.D. Rauh,* EIC Laboratories, Inc.*; A. Burger,* Fisk University*; R.N. Bhattacharyya,* National Renewable Energy Laboratory

This paper describes our recent research in developing highly Li-doped a-Se alloys and thin films for thermal neutron detector applications. The grown Li-doped (35 a/o) a-Se alloy thin films have shown high promise for this application due to the presence of Li in high concentrations, high dark resistivity (2x10@super 14@@ohm@. cm), good charge transport properties (mu-tau@sub e@ = 3.2x10@super -6@ cm@super 2@/V), low cost and relatively easy scale up. Highly Li-doped a-Se alloy has been synthesized in controlled ambient and used for making large area films up to 4x4 sq. inch. The vacuum evaporated a-Se alloy films have been characterized by X-ray diffraction (XRD), atomic absorption (AA), differential thermal analysis (DTA), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). The detectors fabricated from these films have demonstrated potential for thermal neutron detection for the first time. Details of various steps involved in detector fabrication and testing of these devices will also be presented.

5:00pm **SC+EL+SS-WeA10 Instability in Atomic Step Morphology during the Sublimation of Si(111)***, **Y. Homma**, P. Finnie,* NTT Basic Research Laboratories, Japan

A morphological instability has been predicted to occur during step-flow crystal growth.@footnote 1@ Recently we experimentally demonstrated transitions between stability and instability@footnote 2@ during epitaxial growth on an ultra-flat Si(111) terrace - a terrace which is atomically flat on a 100 µm scale. In this paper, we show that such instability can also occur during step-flow sublimation at high temperatures. Step motion due to sublimation was tracked with in situ scanning electron microscopy. When the size of a terrace becomes comparable to the adatom diffusion length, a new step is nucleated, forming the edge of a new, monolayer-deep crater at the center of an ultra-flat terrace. As a result of successive expansion and nucleation, steps become distributed in a concentric circular pattern. The spacing between steps can be controlled by varying the annealing temperature. When the spacing is less than about 20 µm, the innermost step is typically smooth and nearly circular. For larger spacings, the innermost crater is irregularly shaped while it is still relatively small. The crater becomes smoother as it expands. The instability is manifest when the width of the lower terrace is much smaller than that of the upper terrace. Since the adatom flux from a step to a neighboring terrace depends on the terrace width, by reducing the size of the stabilizing terrace the instability can be initiated. The behavior of a subliming surface is thus similar to that of the growing surface. @FootnoteText@ @footnote 1@ G. S. Bales and A. Zangwill, Phys. Rev. B 41 (1990) 5500 @footnote 2@ P. Finnie and Y. Homma, Phys. Rev. Lett. to be published.

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