Pole figure Analysis of GaAs/GaAsSb Nanowire using XRD

Rizwana Kauser[1], ,
[1]Assistant Professor,
Electronics & Telecommunication Department,
DPCOE Pune India

Shanthi Iyer[2]
[2]Senior Research Scientist,
Department of Mechanical and Chemical Engineering,
NCAT State University, Greensboro, NC, USA 27411

Sergey Yarmolenko [3]
[3]Senior Research Scientist,
Department of Electrical and Computer Engineering/Nanoengineering,
NCAT State University, Greensboro, NC USA, 27411

Abstract-**Nanowire (NW) represents an important class of material having the potential to electrically connect the component in an integrated nanoscale and having the two dimensional quantum confinements when smaller than a critical diameter . Nanowires (nanorods or nanowhiskers) have been attracting a great deal of attention as a one-dimensional nanostructure, due to their potential as building blocks for electronic and photonic nanoscale devices. Synthesis of single crystalline semiconductor nanowires has been widely investigated for various materials and methods in particular III-V nanowires have many applications in optoelectronic devices/detectors such as laser, photo diode and detector. Crystal orientation and degree of preferred orientation in nanowire have a great influence on the properties of nanowires. Hence it is crucial for any nanowire based devices to control a preferred orientation texture of nanowires. GaAs /GaAsSb heterostrucure nanowires have been produced using vapor -liquid- solid (VLS) growth mechanism through molecular beam epitaxy (MBE) on silicon (Si) substrate. In particular, epitaxial growth of III-V compound semiconductor nanowires on Si(111) substrates, (despite the substantial lattice mismatch) is very interesting for direct integration of high performance III-V compound semiconductor devices with Si complementary metal oxide semiconductor (CMOS) technology since growth of III-V semiconductor nanowires on Si can solve many problems associated with the large difference in lattice constant and structure. In this paper X-ray diffraction (XRD) analyzes structural and textural properties of GaAs/GaAsSb nanowires by considering pole figure with respect to (220) and (311) orientation planes of grown nanowires.**

Key Words: — Nanowire, XRD, molecular beam epitaxy, gallium arsenide, light emitting diode, pole figure.

1. INTRODUCTION

Recently, semiconductor nanowires are attracting great attention because of their small diameter that leads to one dimensional electron systems and because of being the possibility to be the building blocks of nanoscale electronics and photonics. GaAs/GaAsSb (III-V) nanowire belongs to compound semiconductor family, which possesses large band gap [1] , possibly high emission of light, high electron mobility as well, which can be efficiently used in many electronic applications such as in optoelectronic devices, in lasers and in Light Emitting Diodes etc. Molecular Beam Epitaxy (MBE) is a epitaxial growth mechanism, have been employed to grow GaAs/GaAsSb (111) nanowires on Si (111) substrate under certain conditions, by using VLS (Vapor Liquid Solid) mechanism. Grown nanowire is a single segment nanowire which is having layered structure such as GaAs/GaAsSb/GaAs. Longitudinal growth to achieve abrupt doping profiles or heterojunctions has also been demonstrated by using the VLS method. However, precise control of the sites of nanowires is still difficult unless one resorts to conventional lithographic techniques to position the nanoparticle catalyst. Furthermore, incorporation of catalysts into grown crystals may deteriorate their crystalline quality. Structural analysis is done by Scanning Electron Microscopy (SEM) to show alignment of grown GaAs/GaAsSb (111) nanowire on Si(111) substrate. X-ray diffraction is an important technique in the field of materials characterization to obtain structural information on an atomic scale from both crystalline and non-crystalline (amorphous) materials [2].The X-ray diffraction technique also gives the information about the thickness and roughness, any defects and dislocations present in the sample. An electron in an alternating electromagnetic field will oscillate with the same frequency as the field. When an X-ray beam hits an atom the electrons around the atom start to oscillate with the same frequency as the incoming beam. In almost all directions we will have destructive interference, that is, the combining waves are out of phase and there is no resultant energy leaving the solid sample. However the atoms in a crystal are arranged in a regular pattern, and in a very few directions we will have constructive interference. The waves will be in phase and there will be well defined X-ray beams leaving the sample at various directions which is called diffraction pattern. Hence, a diffracted beam may be described as a beam composed of a large number of scattered rays mutually reinforcing one another.

For diffraction the Bragg's condition should be fulfill which is $2d \sin \theta = n \lambda$ where λ is the wave length of the X-ray beam [3].,θ is the angel of diffraction, d is the interplanery distance between the reflection planes

and n is the order of the diffraction. Here XRD has done with pole figure measurement for different orientations shown in figure [1].The aim of this pole figure representation is to show the orientation of single crystal compared to the orientation of the sample.

Fig-1 Bruker AXS D8 Discover XRD at NCAT,) is used for identification of phases and crystallographic analysis of coatings , using high angle diffraction geometry Ref[5]

A   pole figure is drawn for a specific crystallographic plane (hkl).A point on the pole figure shows the orientation of the normal vector of the (hkl) plane in the reference system. A point on a pole figure corresponds to an orientation of the diffracted or scattering vector K (which is normal to the diffracting plane) in a coordinates system fixed to the sample. When the length of the scattering vector is fixed and a sample is rocked (this situation corresponds to the pole figure measurement and rocking curve measurement) the trajectory of the end of the scattering vector will terrace out a sphere. The pole density for a given point is determined by the intensity of an X-ray beam diffracted for this orientation. The 2theta angle is thus fixed, and the orientation of the sample changes during the measurement. This orientation is described by two angles chi (χ), and phi φ).

　　　　　The   advantage   of   pole   figure measurement with XRD is as follows: Firstly it allows the analysis of textural information of the sample and secondly this measurement can be performed under ambient condition or at low/ high condition by changing the atmospheric condition to find out the textural properties of GaAs/GaAsSb nanowires .In the process of texture analysis of material it is necessary to express the distribution of crystallite lattice in the coordinate of the external fields such as applied stress ,magnetic field etc. For most thin film it would be the lattice of single crystalline substrate [4].

2 EXPERIMENTAL DETAILS.

2.1Diffractometer set up

X-ray data for this research were collected on diffractometer. This instrument was run with Cu X-ray source and a tube power of 40Kv and 40mA, which provide wave length about $1.540562A^0$ .At the source side a beam limiter is used by focusing the incoming X-rays towards the sample Ni filter also used here and at the receiver side to get maximum intensity of diffracted beam we used thin film slit system basically which contains solar slit made up of thin films of copper. The detector as a solid state linear position sensitive detector PSD which allows a scan to be collected in a fraction of the time required with a traditional point detector.

2.2 Characterization

In this research work an epitaxial growth and the structural characterization of GaAs/GaAsSb (111) nanowire on Si(111) substrate is presented . Figure 2 is showing the SEM image of the grown nanowires on substrate. Showing diameter around 170 nm near the base with an average height of 5.9 microns. Average density: .39x10^8 cm-2.SEM image has taken in the range of 2 micromeres. All nanowires have homogeneous diameters and orientation along the wire axis and stand vertically. The grown GaAs/GaAsSb nanowires indicating that they were grown epitaxially on the Si (111) substrate. The crystal structure and crystallinity of the wires was evaluated by the X-ray diffraction (XRD) analysis in the 2θ scan.
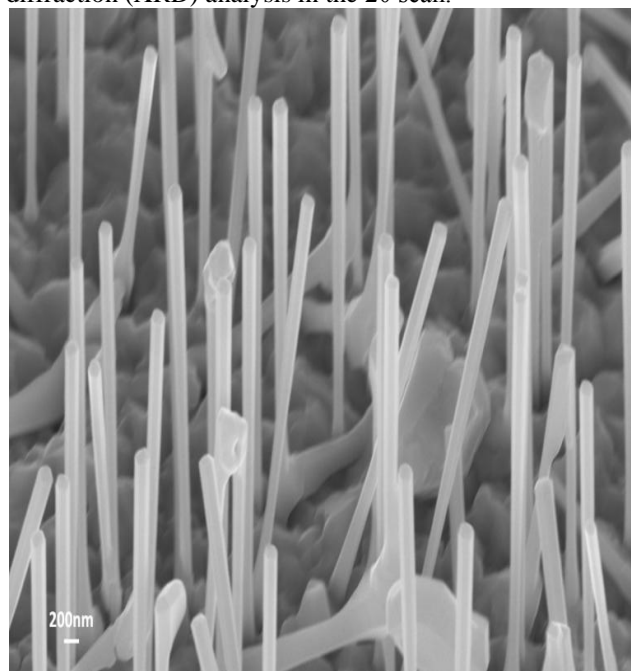

Fig 2 SEM image of GaAs/GaAsSb (111) nanowire on Si (111) substrate.

The vertical alignment of the GaAs/GaAsSb nanowires suggests that there may be an epitaxial crystallographic orientation alignment between the nanowires and substrate. This is substantiated by the initial 2θ XRD scan. Diffracted X-rays always make an angle with the diffraction planes equal to that between the incident beam and diffracted planes. For a standard 2θ (locked coupled) scan, all diffraction will occur from crystallographic planes parallel to the sample surface. Therefore, in 2θ diffraction patterns from a sample of vertically aligned and well oriented nanostructures, the presence or absence of diffraction peaks can give information about the crystallographic orientation of each phase, as well as the growth direction of the nanostructures.
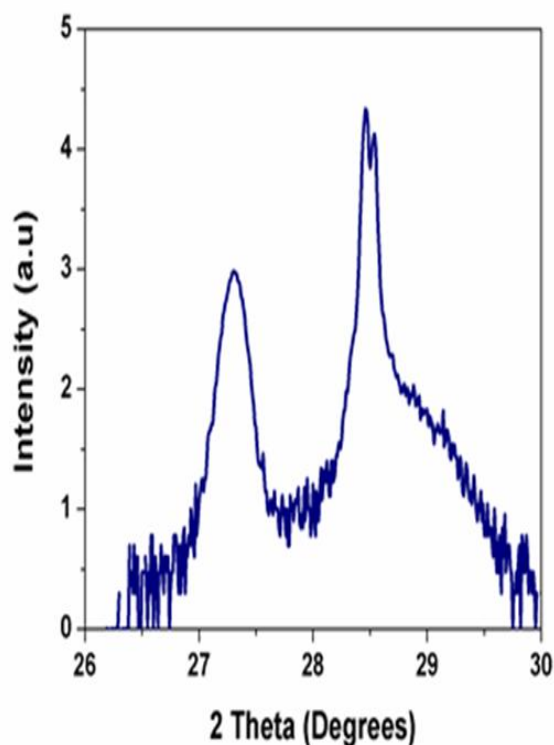

Fig-3 XRD 2-Theta scan of GaAs/GaAsSb nanowire on Si substrate
GaAs/GaAsSb(111) peak at 27.310^0 , substrate Si(111) peak at 28.441^0
and GaAsSb peak at 26.8230 with small intensity

The x-ray diffraction out-of-plane symmetric 2θ scan has done .In 2θ scan there are no significant peaks observed within the whole scan range (from 20^0 to 80^0) except only two peaks one at 27.31^0 for GaAs/GaAsSb (111) and another is at 28.441^0 for the Si(111)substrate as shown in figure 3 . In same figure there is existence of small peak which (not visible) is of GaAsSb at 2θ angle 26.832^0 with low intensity (not visible). In figure locked couple scan indicates that the GaAs/GaAsSb nanowires on a Si (111) substrate are epitaxially grown. In general, the crystal structure of the GaAs/GaAsSb nanowires changes from ZB to WZ or from WZ to ZB through stacking faults along the growth direction [6].

2.3 Rocking curve Measurement

In order to further investigate the crystallographic alignment and to determine the degree of misalignment,(when the length of scattering vector is fixed and the sample is rocked) rocking curves were collected on each phase, as seen in Figure 4 The scan is plotted in terms of theta (θ in Degree) and the intensities are normalized, in order to aid comparisons between the different phase. The full width half maxima (FWHM) value of the rocking curve peak is determined which is 1.4^0 for GaAs/GaAsSb. Generally, during the growth of epitaxial layers of nanowires, each successive layer has a higher degree of misalignment with respect to the central axis, which is indicated by wider rocking curve peaks.
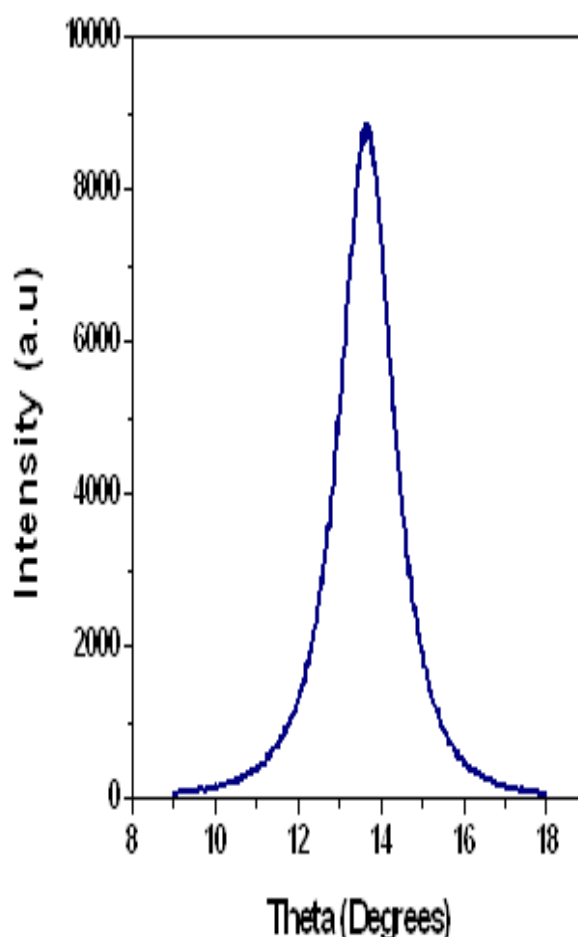

Fig-4 XRD Rocking curve.

2.4 Pole figure Measurement

For more detailed and in depth crystallographic orientation analysis, texture data were collected on vertically aligned ,gallium (Ga) as self-catalyst present on top of the GaAs/GaAsSb nanowires .Pole figure measurement is XRD measurement technique where the diffraction angle 2θ is fixed and the diffracted intensity is collected by varying two geometrical parameters such as χ angel (tilt angle from sample surface normal direction)and azimuthal angle φ angel (rotation angel around sample surface normal

direction). In general centre of the pole figure is defined as $\chi=0^0$ and outer end defined as the $\chi=90^0$. Where φ denotes the rotation angle around the surface normal relative to a certain reference position .It starts at the top of the figure and it is circularly coordinated with counter clockwise direction. Intensity variation along the varying χ with respect to the fixed φ value correspond to the variation due to the tilting motion of the sample. On the other hand the intensity variation along the varying φ with respect to the fixed χ value correspond to the variation to the twisting motion

Nanowires texture data is collected by fixing the X-ray tube (source) and detector to a particular diffraction angle and (this scan is known as locked coupled scan) recording the intensity as the sample is rotated through tilt angle 360^0 φ(phi) and azimuthal angle 90^0 χ(chi) . Figure 5 is showing the XRD full scan Pole figure for {220} reflection plane $\chi=90^0$,$\varphi=360^0$ and $2\theta=43.27^0$ for GaAs/GaAsSb(111) nanowire. Finally, an abbreviated pole figure from the GaAs/GaAsSb{220} reflection was collected before each run in order to align the sample rotation, (The 2θ zero point and sample height, z, were aligned using the standard direct-beam approach.) .For the data analysis, the texture data were plotted in pole figure.
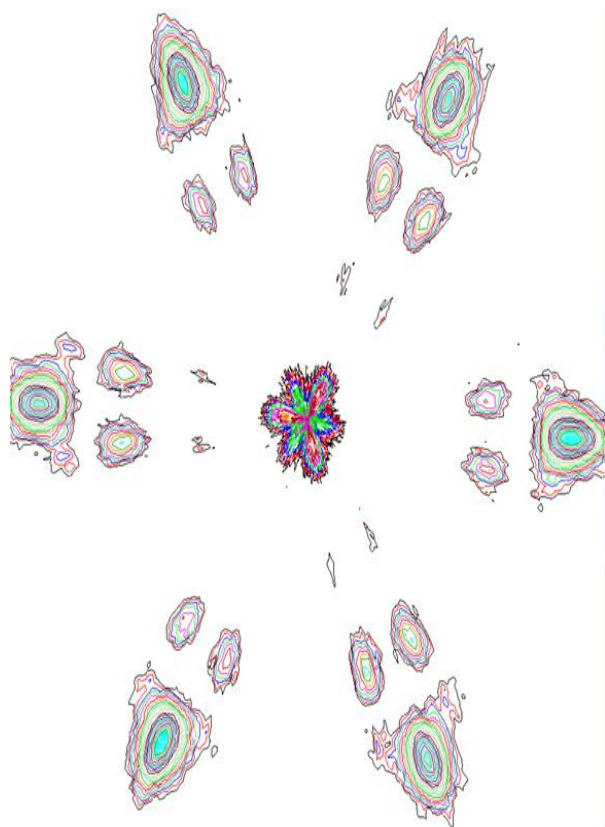
For the sample of vertically aligned GaAs/GaAsSb nanowire (Ga as self catalyst) N1 nanowire texture data were collected on the two reflections plane {220} which showing 50% of the maximum intensity and plane{311} which showing 30% of the maximum intensity for the GaAs/GaAsSb (111) nanowire. The value of 2θ for reflection plane {220} is 43.27^0 , step size has taken 3^0 in φ and χ with a count time of 10 seconds. The value of 2θ for reflection plane {311} is 51.60^0 , step size has taken 5^0 in φ and χ with a count time of 10 seconds. Figure 5 shows the full XRD scan pole figure for GaAs nanowire sample for {220} plane having $\chi=90^0$ $\varphi=360^0$ and $2\theta=43.27^0$.

Figure 6 and 7 are showing the small segment XRD scan for {220} and {311} reflection planes ,showing different constant intensity contours, for $\chi=30^0$,-40^0 and $\varphi=25^0$ -35^0 . At the centre of the contour it is showing highest intensity of the diffracted beam with different color for a small segment.
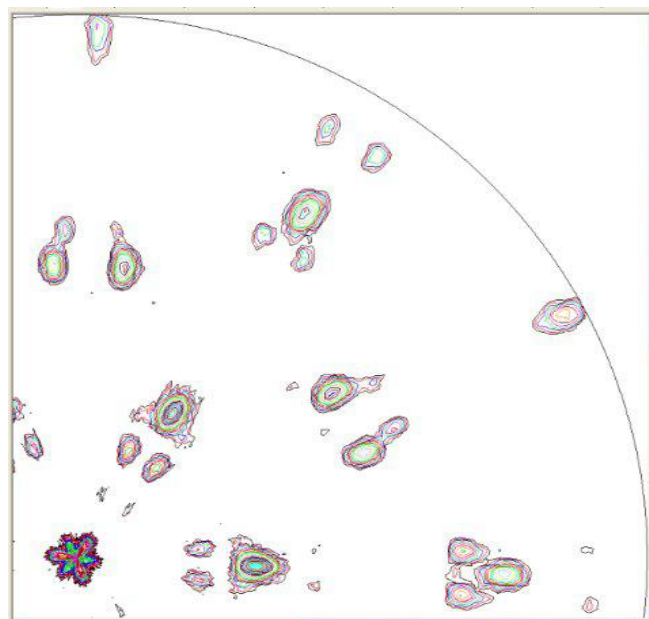

Fig-6 Small segment pole figure for {220} plane

Fig-5 XRD full scan Pole figure for {220} reflection plane χ=90˚, φ=360˚ and 2θ=43.27˚.
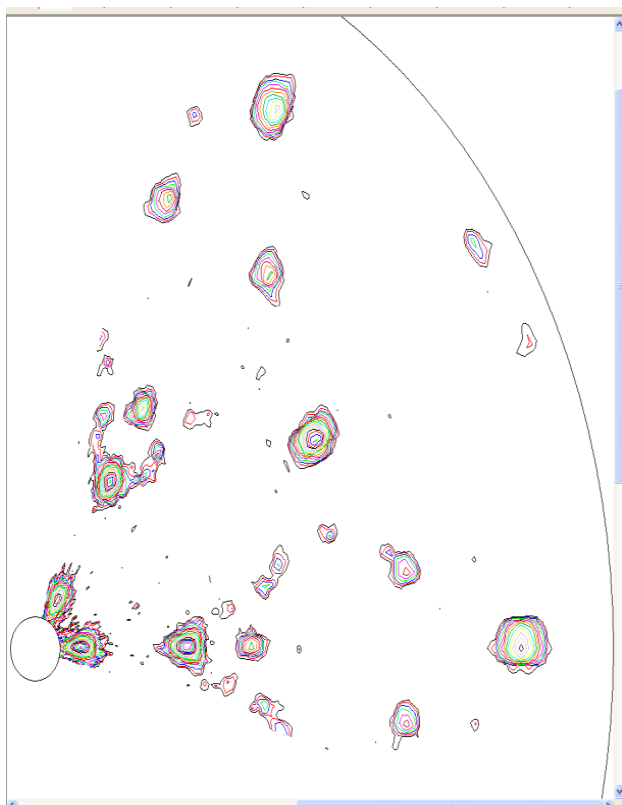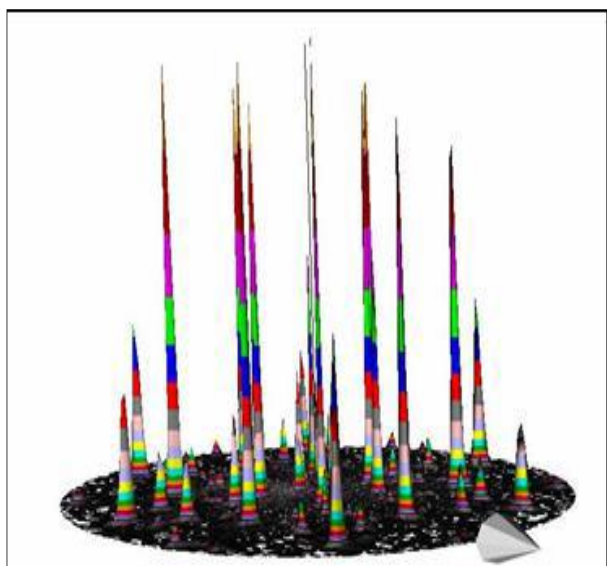
Fig-7 Small segment pole figure for {331} plane

Fig-8 Pole figure in 3D for (220) plane.

Figure 7 is showing the 3D view of full scan pole figure for {220} reflection of the nanowire sample for $\varphi=90^0$ and $\chi=360^0$ and $2\theta=43.27^0$. The 3D view of the pole figure shows that the diffraction intensity peaks including small and larger peaks. The radius of the peak shows the width of each peak, and color in different including small as well as larger peaks corresponds to different value of intensity of the diffraction from the nanowire sample.

2. RESULT AND DISCUSSION

Epitaxial growth of heterostructured GaAs/GaAsSb (111)

nanowires on Si (111) substrate has done. The structural studies presented so far demonstrate that crystalline NI nanowires can be especially grown on a Si substrate, despite the substantial lattice mismatch. As shown in figure 2Cross-sectional SEM image of nanowires confirmed that grown GaAs/GaAsSb (111) nanowires on the Si (111)substrate were vertically aligned and pre-dominantly Oriented along the Si{1 1 1} direction, some other nanowire Orientations were clearly observed.

The nanowire having diameter around 170 nm near the base with an average height of 5.9 microns. Average density is 39x10^8 cm-2.As shown in Figure 3 and figure 4 it is clear that grown GaAs/GaAsSb (111) is having diffraction peak at certain 2θ angle nearly equal to its standard angle value ,which shows that the grown nanowire sample is well aligned and well oriented with respect to the substrate. In order to further investigate the crystallographic alignment and to determine the degree of misalignment of grown nanowires with respect to the central axis .However, the rocking curve peak width is low which is 1.4^0 less than 2°. This small degree of misalignment indicates that the nanostructures grown epitaxially grown and very well aligned. Figure 5 is showing 3 folds symmetry of pole figure analyze that we have to get six larger peaks but due to texture of the sample material is good we are getting larger intensity peak as well as smaller intensity peaks also in the form of constant intensity contours for the reflections {220} and {311}.If we compare pole figure of reflection { 220} (which is showing 50% intensity) and reflection { 311} (showing 30% of intensity), the { 220} reflection showing much batter intensity contour as shown in figures 6 and figure 7.

4. CONCLUSIONS

This paper demonstrates that high quality GaAs/GaAsSb nanowires are epitaxially grown on Si substrate from XRD analysis. The low full width half maxima obtained on the x-ray rocking curve of the (111) plane is reveals high crystalline quality of the grown NWs. XRD full scan pole figure for {220} and {311} reflections exhibited a threefold symmetry. Large intensity and low full width at half maxima are further attest to the high crystal quality of the textured GaAs/GaAsSb NWs. The epitaxially grown nanowires on Si substrate with uniform diameter along the wire axis can provide an opportunity for direct integration of high performance III-V semiconductor nanoscale devices with the well established Si technology.

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