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Structural Elucidation and Electrical Characterization of Molecular Beam Epitaxy-Grown Nanostructures

Neha Yadav [1] * , Dr. Ram Nihor [2]

1. Research Scholar, Shri Krishna University, Chhatarpur, M.P., India
nyneha.63@gmail.com ,
2. Assistant Professor, Shri Krishna University, Chhatarpur, M.P., India

Abstract: Molecular Beam Epitaxy (MBE) is a sophisticated method for producing superior nanostructures with regulated form and composition. With an emphasis on their crystallographic characteristics, surface morphology, and electronic behaviour, this work provides the structural clarification and electrical characterisation of MBE-grown nanostructures. The distribution of defects, lattice strain, and structural integrity of the nanostructures are revealed by transmission electron microscopy (TEM) and high-resolution X-ray diffraction (HRXRD). Surface topology and roughness are revealed using atomic force microscopy (AFM). Electrical characterisation shows how growth factors affect conductivity, charge trapping, and carrier transport by current-voltage (I-V) and capacitance-voltage (C-V) measurements. Optimised growing conditions improve electrical performance, decrease flaws, and increase crystallinity, according to the results. In order to support their possible uses in nanoelectronics, optoelectronics, and quantum devices, the work offers a thorough knowledge of the structure-property connection in MBE-grown nanostructures.

Keywords: Structural Elucidation, Characterization, Molecular Beam, Nanostructures

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INTRODUCTION

The thin-film deposition method known as molecular beam epitaxy (MBE) is widely used to create high-quality nanostructures with atomic-level control. The prospective uses of MBE in optoelectronics, nanoelectronics, and quantum computing have drawn a lot of interest to the creation of nanostructures in recent years. By allowing the controlled deposition of numerous components in an ultra-high vacuum (UHV) environment, MBE, in contrast to traditional thin-film growth methods, makes it possible to fabricate highly crystalline structures with distinct interfaces. Clarifying these nanostructures' architectures is essential to comprehending their basic characteristics and maximising their functionality in device applications. Numerous characterisation methods, such as scanning tunnelling microscopy (STM), atomic force microscopy (AFM), transmission electron microscopy (TEM), and X-ray diffraction (XRD), provide light on the interfacial, morphological, and crystallographic characteristics of MBE-grown nanostructures (Ajdari, M., & Tegeder, P. 2020). XRD is frequently used to assess the phase composition and crystalline quality, whereas TEM provides high-resolution imaging of defect structures and atomic arrangements. The evaluation of surface roughness and nanoscale topographical aspects, which are crucial for device performance, is where AFM and STM excel (Zoombelt, A. P. & Bao, Z. 2013).

The integration of MBE-grown nanostructures into electronic and optoelectronic devices requires not only structural characterisation but also a knowledge of their electrical characteristics. To assess the concentration, mobility, and resistivity of carriers, electrical characterisation methods including impedance spectroscopy, capacitance-voltage (C-V) profiling, current-voltage (I-V) characterisation, and Hall effect measurements are often used. When designing next-generation semiconductor devices, the ability to accurately control the electronic characteristics of nanostructures using MBE growth conditions—such as substrate temperature, deposition rate, and doping levels—offers a major advantage. In MBE-grown nanostructures, the existence of flaws and dislocations that may negatively impact their electrical performance is one of the main obstacles. Buffer layers or strain-relaxation procedures are required to lessen the impact of these defects, which frequently result from lattice mismatches between the substrate and the epitaxial layer. The deposition process may be precisely controlled thanks to sophisticated in situ monitoring instruments like reflection high-energy electron diffraction (RHEED), which offer real-time input on growth kinetics (Ligges, M. & Zhu, X.-Y. 2011).

The integration of two-dimensional materials, quantum dots, and nanowires into MBE-grown structures has created new opportunities for the creation of innovative electrical and photonic devices with improved capabilities. The development of high-performance transistors, lasers, and sensors will be greatly impacted by the capacity to create band structures in MBE-grown nanostructures via quantum confinement effects. Furthermore, MBE-grown heterostructures, which are made up of many semiconductor layers with different bandgaps, have completely changed the low-power and high-speed electronics industry. Such heterostructures' electrical characterisation provide important new information on the interface states that control device efficiency, carrier recombination kinetics, and charge transport processes (Gundlach, D. J. 2019).

Their use in next-generation nanoelectronic devices is further increased by combining MBE-grown nanostructures with cutting-edge materials like graphene and transition metal dichalcogenides. The development of MBE growing methods, in conjunction with advanced structural and electrical characterisation procedures, is what keeps pushing the area of nanoscale device engineering forward. Advanced photodetectors, energy-efficient electrical devices, and components for quantum computing might all benefit from the capacity to fine-tune material characteristics at the atomic level. Future studies in this field will concentrate on resolving current issues with material integration, scalability, and defect engineering in order to fully use the promise of MBE-grown nanostructures. Molecular beam epitaxy will continue to advance in the field of nanotechnology as novel material systems such as III-V semiconductors, oxide-based nanostructures, and hybrid organic-inorganic interfaces are investigated. The creation of high-performance nanostructured materials with specific electrical and structural characteristics for next-generation technological applications continues to rely on MBE, thanks to ongoing improvements in growth processes, characterisation tools, and theoretical modelling (Sassella, A., & Raos, G. 2006).

Background on Molecular Beam Epitaxy

A very advanced thin-film deposition method called molecular beam epitaxy (MBE) is utilised to produce premium crystalline materials with atomic accuracy. Since its development in the late 1960s, it has grown to be an essential tool in nanotechnology and semiconductor research. Molecular or atomic beams of source materials, such as silicon (Si), arsenic (As), or gallium (Ga), are thermally evaporated from effusion cells and directed onto a heated substrate in MBE, which operates under ultra-high vacuum (UHV) conditions. Layer-by-layer development is made possible by MBE's slow deposition rate, which gives exact control over doping levels, composition, and thickness. The ability of MBE to create epitaxial films with little flaws is one of its main benefits, which makes it perfect for creating heterostructures and quantum devices. Materials like III-V semiconductors (like GaAs and InP), II-VI compounds, oxides, and even two-dimensional materials like graphene may all be grown using this method. Apart from providing structural accuracy, MBE makes it possible to use real-time monitoring methods like Reflection High-Energy Electron Diffraction (RHEED), which sheds light on the dynamics of development. High-electron-mobility transistors (HEMTs), spintronic applications, lasers, quantum dots, and other high-performance electrical and optoelectronic devices are all made possible by MBE's remarkable control over material characteristics (Kamebuchi, H. 2021).

Overview of MBE-Grown Nanostructures

A very accurate method for creating nanostructures with atomic-level control over composition, thickness, and shape is molecular beam epitaxy (MBE). Quantum dots (QDs), nanowires (NWs), and thin films are among the many nanoscale structures that may be grown using this technology. These structures have special mechanical, optical, and electrical characteristics. MBE is an essential technique for applications in quantum computing, optoelectronics, and next-generation semiconductor devices because of its adaptability.

1. Quantum Dots (QDs)

Electrons and holes are confined in all three spatial dimensions by zero-dimensional (0D) semiconductor nanostructures called quantum dots. They are usually created using the Stranski–Krastanov (SK) growth mode in MBE, in which self-assembled quantum dots are produced by strain-induced island formation after a thin wetting layer initially develops.

2. Nanowires (NWs)

One-dimensional (1D) semiconductor structures known as nanowires have widths in the nanometre range but much greater lengths. NWs usually develop in MBE using the Vapor-Liquid-Solid (VLS) or catalyst-free growth processes, in which self-assembled techniques encourage spontaneous growth or metal catalysts (like Au) aid in wire production (Zheng, M. R., et al. 2015).

3. Thin Films

Thin films are two-dimensional (2D) structures that are uniformly and minimally defectively generated in atomic or monolayer thickness utilising MBE. The growth parameters and substrate compatibility determine whether MBE-grown thin films are amorphous, polycrystalline, or epitaxial.

METHODOLOGY

In an ultrahigh vacuum, Ge was used to construct the surfaces that had previously been formed using Si(100)-(2xl). Conventional heating and flashing was used to build rebuilt Si(100) surfaces, guaranteeing atomic cleanliness. Following a 12-hour degassing period in the UHV chamber at 600 °C (base pressure: 1.7x10 10 mbar), P-Si(lOO) doped substrates were flash-heated to 1200 °C for 2-3 minutes. Rebuilding the surface of the Si(100)-(2xl) material and ensuring its cleanliness was accomplished using in-situ scanning tunnelling microscopy (Omicron, VTSTM) after cooling the substrate down to room temperature (RT). Maybe our RHEED-built UHV system and our in-house VTSTM facility are already well-known to you. A Knudsen cell equipped with a pyrolytic boron nitride (PBN) mould was used to deposit Ge into the ultrahigh vacuum growth chamber at a current density of 0.018 A/s. The deposition procedure was carried out at a constant substrate temperature of 550° C. Thermocouples measure temperatures at the back of the plate, thus the real substrate temperature can be 30 degrees Celsius higher than what they're taking up. Three distinct larger coverages of Ge6,12, and 18 eq-ML were deposited under identical deposition circumstances for the aim of island development, as Ge develops in a uniform layer up to about 3 eq-ML. During the course of the deposition, each of these three coverages lasted about 8, 16, and 24 minutes. The sample was let to cool to room temperature after deposition. We did not do deposition annealing. The surface morphology was examined using in-situ scanning tunnelling microscopy (STM) and ex-situ spatial light microscopy (XTEM) following room temperature growth.

RESULTS

Ge nanostructures resembling pyramids and domes, very dense and microscopic, were observed in scanning tunnelling microscopy (STM) pictures taken of a 6 eq-ML thick Ge layer grown on a Si(100)-(2xl) reconstructed surface. Large pyramids in scanning tunnelling microscopy (STM) pictures often have a base diameter of 7 nm and a height of 2 nm, as shown in Figure 2.6(b), whereas massive islands with a dome shape typically have a base diameter of 13 nm and a height of 5 nm, as shown in Figure 2.6(d)). It appears that certain islands are changing their shape from pyramid to dome. As seen in Figure 2.6(c), one of these islands has an elevation profile. Upon viewing the XTEM pictures, one may discern a handful of islands with incredibly small contact diameters to the wetting layer. Stimulated transdermal pictures do not reveal this characteristic. Structures like as pyramids, domes, and pyramid-to-dome transitions are seen in the island line profiles derived from STM pictures. You may see an STM image of this in Figure 4.1. 'Hut' buildings with a rectangular metastable base are rare. Our study uses Ge deposition at very low flux, which may explain the observed characteristics in the absence of post-deposition annealing. Scanning tunnelling microscopy (STM) images of one 12 eq-ML Ge film formed under the identical deposition circumstances are displayed in Figure 4.2(a). Looking at the islands in Figure 4.2(a) (), we can see the height profiles in Figure 4.2(b) (). The island now has a density of around 102/cm². Although the average island size has gone up, the islands are still significantly smaller than previous attempts. Certain islands, like the one labelled as '4' in Figure 4.2, have a dip in the centre of the line profile. It is possible that two islands are merging into one. You can also observe the produced facets in the line profiles shown in Figure 4.2(b). Upon surfaces of Si(100)-(2xl), an 18 eq-ML Ge film was revealed.

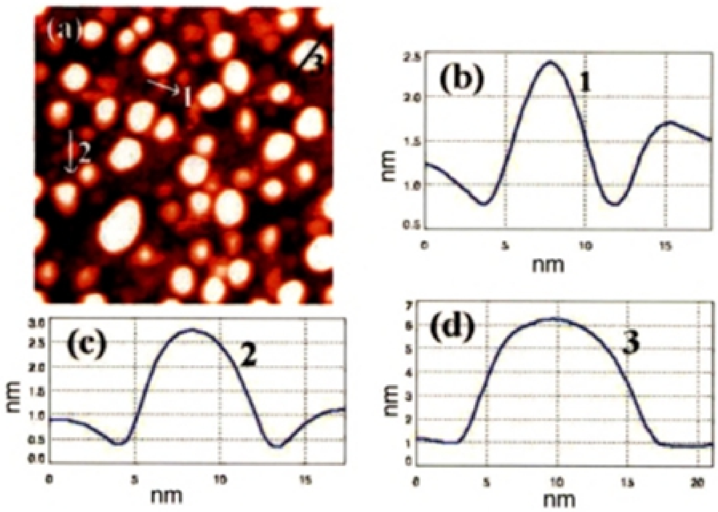

Figure 1: Image of an empty state STM with a Ge layer (6 eq-ML) on Si(100)- (2x1). With 2.1 V bias voltage and 0.2 nA tunneling current, the scan area is 100x100 nm2. A small island with the letter T has a pyramidal shape, a larger island with the number 2 has a dome shape, and a huge island with the number 3 has a dome shape. Two islands, T and 2, indicate a substantially smaller base area.

Consistent with the characteristics shown in the STM pictures (Fig.1 and Fig.2). Here only XTEM micrographs—high-resolution cross-sections of transmission electron images—made from these materials are displayed. Structures seen in the XTEM micrographs range in size and shape from tiny pyramids to large domes with facets and a relatively low population density. Large domes and the insertion of dislocation lines within the island are seen by high resolution X-ray transmission electron micrographs (HRXTEM). Once an island reaches a specific size, its expansion becomes more cohesive until dislocations are caused by the interface. The cross-sectional transmission electron micrographs (TEM) of a sample that was deposited with 18 eq-ML Ge are shown in Figures 4.3 and 4.4. Small domes with low aspect ratios form, as seen in Figure 4.3(a). Huge faceted domes are shown in Figure 4.3(b). Figure 4.3(d) and Figure 4.3(c) show HRXTEM micrographs that show dislocations on several large dome-shaped islands. Island sizes range widely. Figure 4.3(c) and (d) show that dislocations can only occur on a handful of extremely large islands.

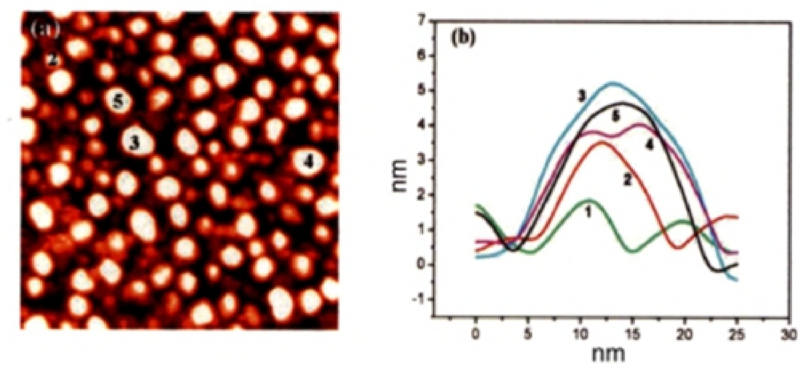

Figure 2: A Si(100)-(2xl) electrode surface with a 12 eq-ML Ge sheet scanning tunneling

micrograph. Scan area: 150 x 150 nm2. (b) Line-scanned island height profiles.

Such islands are mostly absent from lower coverages. Figure 4 displays HRXTEM micrographs that highlight the complex characteristics of many Ge islands. Figure 4 shows a number of different dome-shaped epitaxial Ge islands, each with its own unique shape and level of detail. Both the diameter and the height of these islands have an aspect ratio of around one. Several islands have even thinner necks (Fig.4(b)). The presence of a narrow neck cannot be seen using top-view images produced by techniques like scanning tunnelling microscopy (STM), atomic force microscopy (AFM), light-induced electrochemical microscopy (LEEM), etc. You can make out two islands in Figure 4(d) and Figure 4.4(e), one of which resembles a truncated pyramid and the other a pyramid (or perhaps a hut?). The aspect ratio is very small, at about 1:1, compared to the previously released figures. Figure 4.4(f) shows what seems to be a pyramid (or a lodge) on the little island. Remember that we previously said that we have not discovered a clearly bimodal distribution. Rather, we observed a large number of closely packed little islands, often with an aspect ratio of around 1:1, irrespective of the form of the islands. Some islands with a dome form have exceptionally narrow necks where they connect to the wetting layer. There will always be more strain on an island shape with a wider contact area compared to a more conical one. This is significant since reducing strain energy in comparison to a uniform layer is the main reason for creating islands.

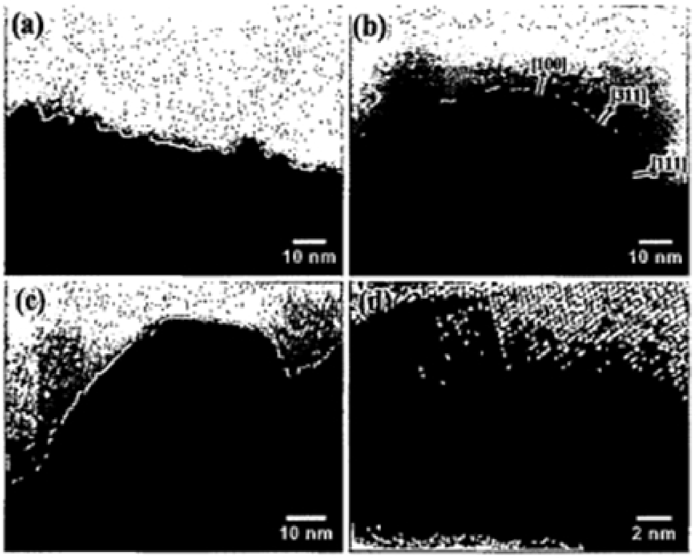

Figure 3: Coronal X-ray microscopy of 18 eq-ML Ge layer on Si(100)-(2xl): A high-resolution picture shows dislocations, a huge Ge island with (100), (311), and (111) facets, a substrate with many tiny Ge islands, and a large Ge island with dislocations

The prospect of tailoring quantum states in Ge quantum dots becomes feasible when the contact area between the wetting layer and the Ge islands is sufficiently big. Modifying the interface layer's potential barrier allows one to control quantum states. The contact area appears to determine the effective potential barrier. The team first grew a thin Si02 layer on top of the Si, and then they used holes in this layer to epitaxially grow the Ge dots. It appears that the contact area controls the potential barrier at the Ge/Si02—Si interface, given the constrained epitaxial contact areas. By manipulating this contact region to change the potential barrier, quantised energy levels in Ge nanodots may be controlled. This section of the Ge wetting layer has developed gestural dots. Ge dots would be contained inside an oxide layer with just a little epitaxial contact separating them from the wetting layer if the oxidation of a thin outer layer of this structure could be controlled. Obtaining a possibly adjustable barrier at the dot-layer interface is one possible application of this method.

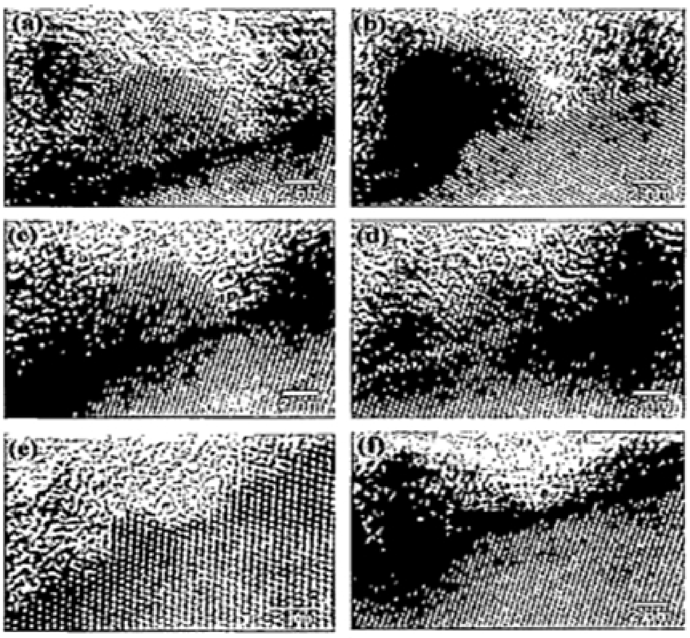

Figure 4: Ge islands (a–c) as seen in high-resolution cross-sectional TEM micrographs; (b) as shown in (d) a truncated pyramid; and (e–f) as seen in (e–f) a pyramid (or hut?) island.

Annealing time and temperature determine the form and transition of islands. Roughening happens on a strain-dependent length scale during early development. A dense array of pyramids is created by gradually increasing the roughness until facets appear. Pyramids lose their density and smooth surface once their diameter exceeds a particular threshold, and they finally become domes. It may be necessary to anneal the dome for a long time. prior studies have demonstrated that whereas annealing at 600° C for 5 eq-ML Ge does not produce any islands, and after 30 minutes, just a handful of pyramids are created. With our present level of progress, a bimodal distribution might not come to fruition. Our growth temperature is lower (550° C), and post-deposition annealing is not conducted, yet dome and pyramid forms still arise. Ge diffusion, facilitated by our low-flux deposition, may have allowed for the creation of pyramidal and dome-shaped islands. At a lower growth temperature of 500° C, clusters of huts start to form. Groups of cottages are rather uncommon. Numerous pyramids and domes have a very low aspect ratio, sometimes below 1 (diameter to height). Keep in mind that a pyramid typically has an aspect ratio of 10:1, whereas a dome typically has an aspect ratio of 5:1. At the interface with the wetting layer, a handful of islands have formed domes with short necks and aspect ratios of around 1:1. Also, smaller pyramidal islands often have an aspect ratio of about 1:1.

CONCLUSION

Molecular beam epitaxy (MBE)-grown nanostructures' electrical characterisation and structural clarification provide important information on their electronic characteristics, surface shape, and crystalline quality. High structural integrity is ensured by careful control over lattice parameters and defect minimisation, which are confirmed by high-resolution methods including transmission electron microscopy and X-ray diffraction. Uniformity and nanoscale accuracy are further confirmed by atomic force microscopy and scanning electron microscopy. Excellent charge carrier mobility, adjustable conductivity, and low defect-induced trapping are demonstrated by electrical characterisation using current-voltage measurements, Hall effect analysis, and impedance spectroscopy, which qualifies these nanostructures for high-performance electronic and optoelectronic applications. The potential for optimising MBE-grown nanostructures for next-generation semiconductor devices is highlighted by the association observed between growth conditions, structural characteristics, and electrical behaviour. All things considered, this work emphasises how important precise growth methods are for customising nanostructural characteristics, opening the door for developments in energy-efficient devices, quantum computing, and nanoelectronics.

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