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Ge Growth on Pure SI (100) Surfaces: Minuscule Ge Islands With Low Aspect Ratio of Diamter to Height

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ABSTRACT

Self-assembled Ge nanostructures on Si(100)-(2×1) were grown by low-flux molecular beam epitaxy at 550°C without annealing. Ge coverages of 6, 12, and 18 eq-ML were studied by in-situ STM and ex-situ HRXTEM to examine island formation beyond the 3 ML wetting layer. A dense array of low-aspect-ratio islands ~1:1 was observed, unlike typical pyramids ~10:1 and domes ~5:1. Island density reached ~10^{12} cm^{-2} at higher coverage, with shapes including truncated pyramids and faceted domes. Most islands remained coherent. Low flux enhanced diffusion and suppressed coarsening, yielding defect-free islands. This approach may enable control of interfacial barriers for Si-based quantum dot devices.

KEYWORDS

Ge/Si heteroepitaxy, Stranski-Krastanow, quantum dots, STM, TEM, low aspect ratio

INTRODUCTION

Over the last decade, semiconductor nanostructures have grown in popularity for many different reasons. Their structural and electrical characteristics are rich, and they allow one to artificially synthesize semiconductor carrier, electron, and hole potentials on length scales less than or equal to the de Broglie wavelength. From both a scientific and practical standpoint, semiconductor nanostructures are of great interest. Quantum confinement effects may be controlled to a large extent and so play a crucial role. Many previously only accessible as simplified theoretical models may now have their properties investigated thanks to the advent of semiconductor nanostructures. those of practical significance and those of scholarly curiosity can both benefit from quantum mechanics. Novel idea devices are made possible by quantum confinement phenomena.

The application of semiconductor nanostructures in opto and nano-electronics is thus highly promising. The earliest systems that match a fundamental theoretical model, such a quantum well or a one-dimensional potential variation, were heterostructures generated epitaxially. Stacks of planar layers of different semiconductors make up these structures, which are possible variants along the growth route. But the highest bound of low-dimensional structures is the quantum dot, a structure with carriers restricted in all three dimensions. If the desired

electrical properties are to be achieved, dot interfaces must likewise be free of defects. The structural sizes of most semiconductor devices, which are typically on the order of 10 nm, make them challenging to fabricate using standard methods. Despite advancements in nanostructure construction using techniques like electron beam lithography, there is still a considerable distance to travel before modern manufacturing methods can deliver defect-free interfaces.

We started by talking about and looking at island formation in heteroepitaxial ionic crystals. We have just realized that islands forming on wetting layers in heteroepitaxial systems with different lattice constants, as In As/GaAs or Ge/Si systems, may be made into zero-dimensional semiconductor nanostructures. For this occurrence, the Stranski-Krastanow (SK) development mode was appropriate. The finding that, under optimum growth circumstances, the size distribution (height vs. lateral size) may be greatly limited allowed for a more reliable evaluation of the optical characteristics of quantum dots and reduced inhomogeneous line widening. Devices like injection lasers, which have some advantages over strained III-V quantum well systems, might be made using the quasi-zero-dimensional density of states in InAs islands implanted in GaAs.

We have developed densely inhabited islands with a restricted size range for diverse combinations of materials in our numerous attempts to understand and manage self-organising development processes. In addition, methods for constructing islands by lateral attachment have been discovered, and self-assembled islands have transitioned from a fascinating field of basic research to a crucial component of several devices.

The SK mode is one of the most prominent modes of development for this technique. Nanoscale islands are created when a two-dimensional (2D) wetting layer is utilised to promote an increase in semiconductor heterostructures with a certain lattice mismatch. Although this could change with the introduction of new devices that use Ge/Si heteroepitaxial layers, the indirect band gap of silicon makes optoelectronic applications impractical for Si devices at the mo ment. An optimal arrangement for such uses would consist of a dense cluster of tiny islands with a very narrow size distribution. Conventional lithography techniques are unable to accomplish the exceedingly tiny island sizes required to generate confinement effects at room temperature.

Germanium (Ge) may spontaneously self-assemble into three-dimensional islands when grown epitaxially on silicon (Si). Stress in the pseudomorphic Ge film causes this phenomenon, which is a result of the 4.2% lattice mismatch between Ge and Si. Competition between surface energy and strain energy causes the creation of 3D islands, which partially relieve the accumulated strain, until the Ge coverage surpasses 3 monolayers (ML). These islands change their shape in a variety of ways as they expand. Their original shape on a Si(100) surface is that of squares or rectangles called "hut clusters." Pyramids and domes are among the other forms. These islands can either be coherent (free of dislocations) or have misfit dislocations, the latter of

which drastically lower strain energy in bigger islands. Usually, the islands self-assemble at the nanoscale via the Stranski-Krastanov (SK) growth mode. The Ge-Si lattice mismatch provides unique obstacles, and this technique offers an alternate way to overcome them. The strain distribution in a developing sample determines the surface nanostructures and how they are arranged with each other. The end result is very regular ensembles of nanostructures spanning a small size range that form stunningly flawless one-, two-, or even three-dimensional lattices.

As an example, a strain field might form as a result of minor islands situated underneath the layer upon which the next layers are constructed. One novel approach to creating self-organising semiconductor nanostructures has been to grow Ge atop amorphous nitride sheets with microscopic pores. This would pave the way for the Ge islands and Si substrate to form an epitaxial connection. Recent findings indicate that surfaces with Si(111)-(7x7) oxidation can support a multitude of epitaxial Ge nanoislands. These tiny, spherical nanoislands feature fragile neck connections and are less than 10 nm in size. Once further, the oxide layer is heated to a point where tiny holes are formed, therefore attaining the epitaxial relation. The growth of nanostructures is not, however, predicated by the Frank-van der Merwe mechanism of layer-by-layer epitaxy. A step bunch can be generated by the interaction of the steps in a two-dimensional layer's expansion in a step-flow regime. The direction of substrate surface misorientation with respect to the ideal crystallographic surface orientation determines whether the step bunches break into a zigzag pattern or not; even in homoepitaxy, tiny zero-dimensional structures can emerge. A one-dimensional nanowire may be produced in a multilayer structure, such as Si/Ge/Si, by the selective aggregation of Ge at these step bunches. Before delving into epitaxial Ge growth on Si surfaces, we will swiftly examine several instances of non-epitaxial (self-assembled) Ge nanostructure creation.

These structures may be created by using high vacuum deposition on passivated surfaces. Under a high vacuum, surfaces of silicon oxide, regardless of cleanliness, oxidise rapidly. Evidence from theory and experiment points to the possibility that halogens and other monovalent elements can inhibit oxidation during adsorption by passivating surface bonds that are dangling. The possibility of epitaxial growth of self-assembled structures on passivated Si surfaces has been demonstrated before.

One potential result of depositing Ge on passivated Si substrates is the formation of self-assembled Ge nanoislands. Nanodots are deposited on the Ge layer by a layer-to-island mass transfer method. With an activation energy for surface diffusion as low as 0.45 eV, X-ray reflectivity tests even at ambient temperature demonstrated that Ge surface diffusion was considerable. By depositing Ge onto Si surfaces coated with polymers, Ge nanowires and nanodots were created using this data.

METHODLOGY

A Ge material was used in an ultrahigh vacuum to recreate surfaces that had previously been manufactured using Si(100)-(2xl). The standard heating and flashing approach was used to manufacture rebuilt Si(100) surfaces, guaranteeing atomic cleanliness. Substrates doped with P-Si(lOO) were degassed in the UHV chamber at 600 °C for 12 hours (base pressure: 1.7x10 10 mbar) before being flash-heated to 1200 °C for 2-3 minutes. After bringing the substrate down to room temperature (RT), we employed in-situ scanning tunneling microscopy (Omicron, VTSTM) to rebuild the surface of the Si(100)-(2xl) material and ensure that it was clean. Perhaps you're already familiar with our in-house VTSTM facility and the RHEED-built UHV system we developed. The ultrahigh vacuum growth chamber was used to deposit Ge at a current density of 0.018 A/s from a Knudsen cell equipped with a pyrolytic boron nitride (PBN) mold. A substrate temperature of 550° C was maintained throughout the deposition process. (The actual substrate temperature can be up to 30 degrees Celsius greater than what the thermocouple is picking up since it's measuring the temperature at the back of the plate). Since Ge develops in a uniform layer up to around 3 eq-ML, three different greater coverages of Ge 6, 12, and 18 eq-ML were deposited under similar deposition conditions for the purpose of island development. All three of these coverages took about 8, 16, and 24 minutes throughout the deposition process. Following deposition, the sample was allowed to cool down to room temperature. No deposition annealing was performed. Analysis of surface morphology after room temperature growth was carried out using in-situ scanning tunneling microscopy (STM) and ex-situ spatial light microscopy (XTEM). To determine how much Ge was deposited during growth, the quartz crystal's thickness was measured. The thickness monitor was previously calibrated for different amounts of Ge deposition and growth rates using data from Rutherford backscattering spectrometry (RBS). We can get the deposition rate by finding the slope of the linear relationship between thickness and deposition time.

RESULTS AND DISCUSSIONS

Scanning tunneling microscopy (STM) images of a 6 eq-ML thick Ge film grown on a Si(100)-(2xl) reconstructed surface show the formation of Ge nanostructures in the shape of pyramids and domes, which are relatively dense and very small. Typical dimensions for large pyramids in scanning tunneling microscopy (STM) images are 7 nm in base diameter and 2 nm in height Figure 1(b), where as huge islands shaped like a dome usually have 13 nm in base diameter and 5 nm in height Figure 1(d). Seemingly, the form of certain islands is shifting from pyramid to dome. An elevation profile of one of these islands is shown in Figure 1(c). After the XTEM images are shown, you may be able to make out a few islands that have a very tiny contact diameter to the wetting layer. This feature is not seen in stimulated transdermal images. The line profiles of the islands, which are obtained from STM images, display pyramid, dome, and

pyramid-to-dome transition structures. An STM picture of this may be shown in Figure 1 'Hut' structures with a metastable rectangular base are unusual. Perhaps the observed properties in the lack of post-deposition annealing can be explained by our work's use of Ge deposition at very low flux. One 12 eq-ML Ge film grown under the same deposition conditions is shown in Figure 2 (a) as a scanning tunneling microscopy (STM) image. Figure 2 (b) shows the height profiles, which can be seen from the islands in Figure 2 (a) . Density on the island has increased to around 102/cm². In spite of an increase in the average island size, the islands remain much smaller than in earlier efforts. A dip in the middle of the line profile is seen on certain islands, such as the one shown as '4' in Fig.2. Two islands might be converging into one. The generated facets may also be seen in Figure 2 (b)'s line profiles. Upon Si(100)-(2xl) surfaces, an 18 eq-ML Ge film disclosed.

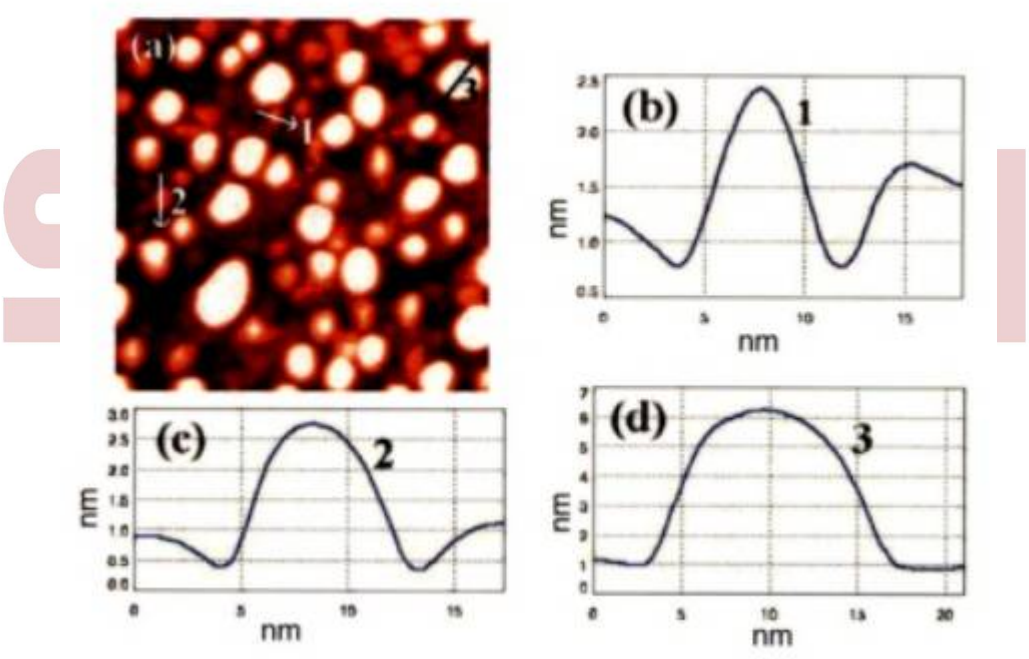


Figure 1: Image of an empty state STM with a Ge layer (6 eq-ML) on Si(100)- (2x1). With 2.1 V bias voltage and 0.2 nA tunneling current, the scan area is 100x100 nm². A small island with the letter T has a pyramidal shape, a larger island with the number 2 has a dome shape, and a huge island with the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

Match the traits seen in the STM images Figure 1 and Figure 2. Only XTEM micrographs, which are high-resolution cross-sections of TEM pictures, derived from these materials are shown here. The XTEM micrographs show a variety of shapes and sizes of

structures, including small pyramids, truncated pyramids, domes, facetted domes, and huge domes (very low population density). High resolution X-ray transmission electron micrographs (HRXTEM) reveal large domes while also revealing the introduction of dislocation lines within the island. When islands reach a certain size, they begin to expand in a cohesive fashion until the interface begins to cause dislocations. Figures 3 and 4 provide transmission electron micrographs (TEM) taken cross-sectionally of a sample that underwent 18 eq-ML Ge deposition. In Figure 3(a), little domes with low aspect ratios are shown to develop. Figure 3(b) shows a large faceted dome. Both the HRXTEM micrograph in Figure 3(d) and Figure 3(c) demonstrate the presence of dislocations on many massive dome-shaped islands. The size of islands varies greatly. Dislocations are limited to a small number of very large islands, as seen in Figure 3(c) and (d).

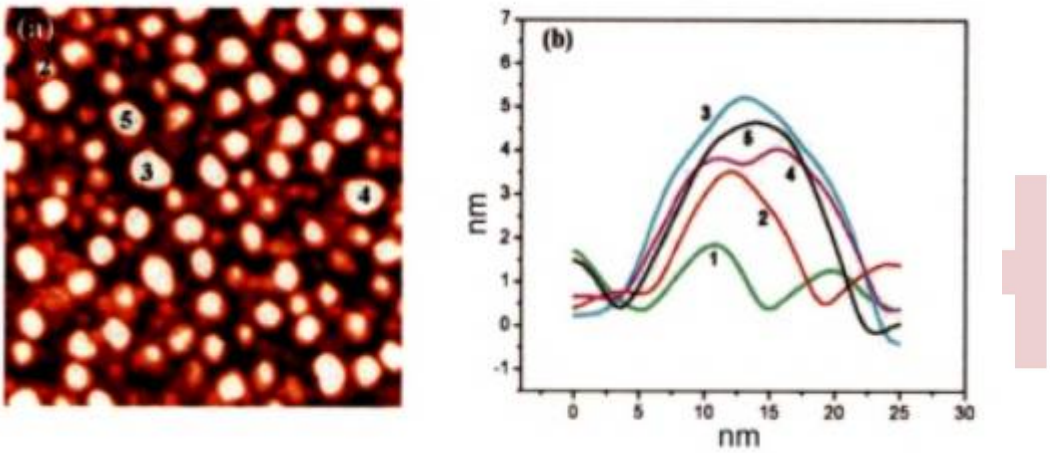


Figure 2: A Si(100)-(2xl) electrode surface with a 12 eq-ML Ge sheet scanning tunneling micrograph. Scan area: 150 x 150 nm². (b) Line-scanned island height profiles.

Lower coverages are largely devoid of such islands. In Figure 4, we provide HRXTEM micrographs that illustrate the intricate features of a few Ge islands. Various dome-shaped epitaxial Ge islands with varying form details are shown in Figure 4[(a), (b) and (c)]. The aspect ratio of these islands is about one for both diameter and height. Even more thin necks may be seen on several islands □Figure 4 (b)□. Techniques such as scanning tunneling microscopy (STM), atomic force microscopy (AFM), light-induced electrochemical microscopy (LEEM), etc., yield top-view pictures and hence cannot identify the existence of a narrow neck. Two islands, one with a pyramid shape (or maybe a hut?) and the other looking like a truncated pyramid, may be seen in Figure 4 (d) and Figure 4 (e), respectively. Once again, the aspect ratio is tiny, at around 1:1, in comparison to the numbers that were previously published. It seems like a pyramid (or a cabin) on the little island in Figure 4 (f). We have already stated that there is no evidence of a bimodal distribution. We found instead a preponderance of densely packed little

islands, with an aspect ratio of around 1:1 in many instances, regardless of island shape. At the point where they meet the wetting layer, the necks of certain dome-shaped islands are rather thin. Island shapes with a broad contact surface naturally cause more strain than those with a more conical form. Because the primary motivation for island creation is to lower strain energy relative to a uniform layer, this becomes important.

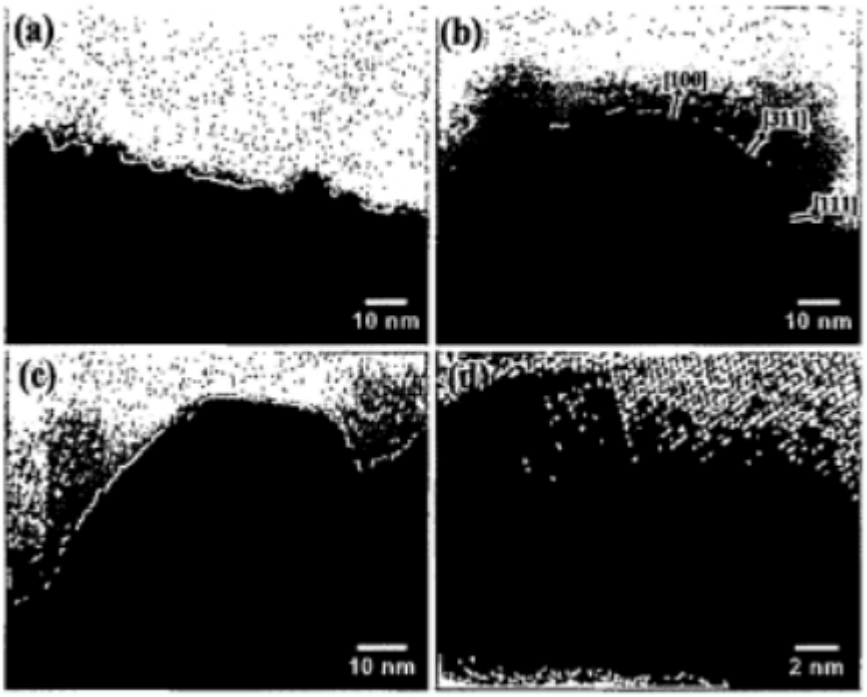


Figure 3: Coronal X-ray microscopy of 18 eq-ML Ge layer on Si (100)-(2xl): A high-resolution picture shows dislocations, a huge Ge island with (100), (311), and (111) facets, a substrate with many tiny Ge islands, and a large Ge island with dislocations

A large enough contact area between the wetting layer and the Ge islands opens the door to the possibility of customizing quantum states in Ge quantum dots. One may manipulate quantum states by adjusting the potential barrier of the interface layer. The effective potential barrier seems to be dependent on the contact area. Their process included growing a thin Si02 layer on top of Si, and then creating the Ge dots epitaxially via holes in the Si02 layer. Given the restricted epitaxial contact regions, it seems that the contact area determines the potential barrier at the Ge/Si02—Si interface. It will be possible to manage the quantized energy levels in Ge nanodots by modifying this contact area to alter the potential barrier. Gestural dots have formed

in this area of the Ge wetting layer. If the regulation of the oxidation of a thin outer layer of this structure could be achieved, Ge dots would be enclosed in an oxide layer with just a little epitaxial contact separating the wetting layer from the Ge dot. It is believed that this method may be employed to obtain a dot-layer interface barrier that could be adjusted.

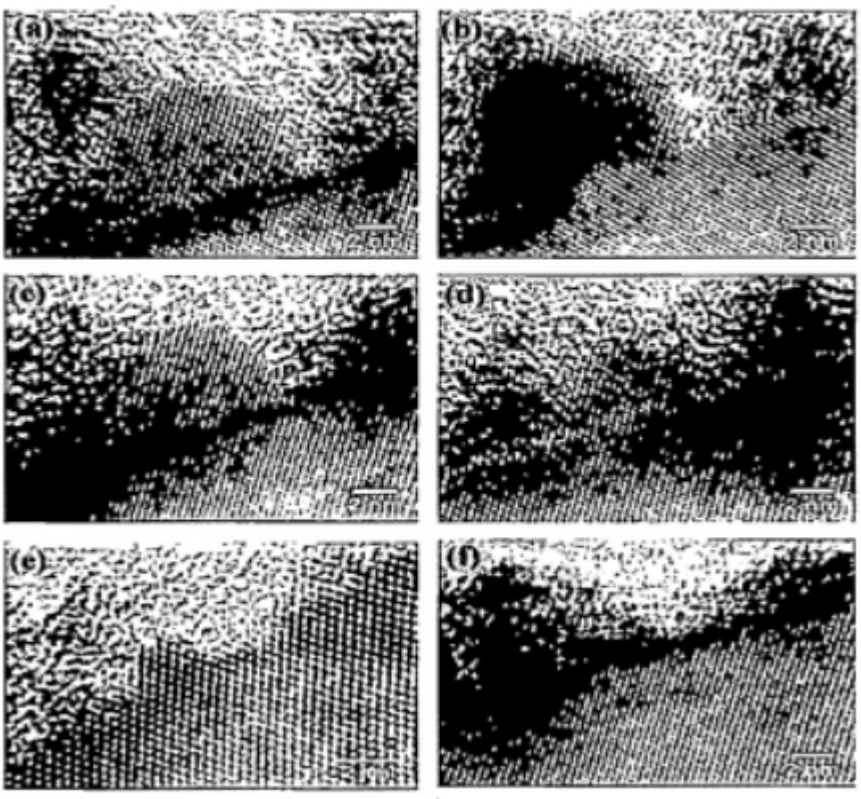


Figure 4: Ge islands (a–c) as seen in high-resolution cross-sectional TEM micrographs; (b) as shown in (d) a truncated pyramid; and (e–f) as seen in (e–f) a pyramid (or hut?) island.

The shape and transition of islands are influenced by annealing temperature and duration. Roughening occurs during early development on a length scale that depends on strain. In the process of creating a dense array of pyramids, the roughness increases until facets emerge. As their diameter increases beyond a certain point, pyramids become less dense and rougher, eventually transforming into domes. The dome could need annealing over an extended period of time. Prior studies have demonstrated that no islands are produced prior to annealing at 600° C for 5 eq-ML Ge, and only a few of pyramids are produced after 30 minutes. A bimodal distribution may not materialize given our current state of development. Dome and pyramid structures emerge even though our growth temperature is lower (550° C) and post-deposition annealing is not performed. Perhaps the formation of pyramidal and dome-shaped islands is

enabled by Ge diffusion due to our low-flux deposition. Clusters of huts begin to take shape at a lower growing temperature of 500° C. Rare are groupings of huts. Pyramids and domes frequently have an aspect ratio below 1, meaning their diameter is less than their height. Remember that the aspect ratio of a pyramid is usually 10:1, whereas that of a dome is usually 5:1 A few islands have developed domes with narrow necks at the interface with the wetting layer and aspect ratios of around 1:1. In addition, the aspect ratio of smaller pyramidal islands is around 1:1.

CONCLUSION

In this work, self-assembled Ge quantum dots were grown on Si(100)-(2×1) surfaces by molecular beam epitaxy at a low substrate temperature of 550°C and a low deposition flux of 0.018 Å/s without any post-deposition annealing. The growth of Ge islands was studied for coverages of 6, 12, and 18 eq-ML using in-situ STM and ex-situ HRXTEM.Our results show that even at low temperature and low flux, both pyramidal and dome-shaped islands coexist from the initial stage of island formation. The islands obtained are significantly smaller in size compared to previously reported data. At 6 eq-ML coverage, pyramids with ~7 nm base diameter and 2 nm height, and domes with ~13 nm base diameter and 5 nm height were observed. A key finding is the presence of a large number of densely packed islands with a low aspect ratio of ~1:1 and, in some cases, a thin neck at the interface with the wetting layer. This morphology is typically not observed without annealing and is attributed to limited surface diffusion at low flux.With increasing coverage to 18 eq-ML, the island density increased to ~10^11 cm^-2. The aspect ratio remained low for most islands. HRXTEM analysis revealed that dislocations appear only in very large dome-shaped islands, while smaller pyramids and domes remain coherent. No clear bimodal size distribution was observed.The absence of post-growth annealing combined with low flux deposition appears to suppress Ostwald ripening and allows for the formation of small, dense Ge islands directly during growth. This approach provides a route for fabricating minuscule Ge quantum dots on Si(100) with controlled size and shape, which is promising for CMOS-compatible optoelectronic and nano-electronic device applications.

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