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# Direct measurement of strain in a Ge island on Si(001)

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We report on a direct measurement of the strain in a single Ge ''quantum dot'' island grown on Si by chemical vapor deposition. This transmission electron microscopy method is reliable: without the need for detailed modeling of the strain field, it measures the maximum in-plane displacement. Good agreement is found between the experimental value of $0.86\pm0.17\%$ average strain and finite element simulations assuming pure Ge. Thus no evidence of significant alloying with Si is observed.
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In recent years, researchers have shown considerable interest in Ge–Si heteroepitaxy due to the system's potential technological importance and to basic questions regarding the system's morphological evolution. The observation that Ge forms uniformly sized, nondislocated, well-ordered arrays of islands when deposited under appropriate conditions onto Si(001)[1–3] has led to the hope that this simple system will find applications in novel electronic and optical devices. Alternatively, several aspects of this system's morphological evolution have led to differing theories regarding the mechanism of evolution, including the basic question of whether the different morphologies arise kinetically or thermodynamically.[4–6] Since the lattice parameter of Ge is 4.2% larger than that of Si, strain is an important feature of the system and plays a key role in the system's behavior, both electronically and morphologically.

Transmission electron microscopy (TEM) has long been recognized as a valuable tool for measuring strain;[7,8] the challenge is finding a simple way to model complicated strain fields. Below, we show that a universal strain model can be used to measure strain due to Ge quantum dots and many related systems.

The islands analyzed were deposited by chemical vapor deposition on Si(001) wafers. After baking at 1150 °C in a $H_2$ ambient and depositing a Si buffer layer at 1080 °C, Ge was deposited at 600 °C and a pressure of 10 Torr using $GeH_4$ in a $H_2$ carrier gas. The amount of Ge deposited was equivalent to 11 ML ($1\ \mathrm{ML}=6.27\times10^{14}\ \mathrm{Ge\ atoms\ cm^{-2}}$). The heating power was turned off shortly after the $GeH_4$ flow stopped, and the sample was not intentionally annealed. Further details of the growth can be found elsewhere.[3] We prepared TEM specimens by mechanical dimpling followed by wet chemical thinning in a 1:10 HF:$HNO_3$ solution. Wax which was applied to protect the Ge-coated surface from the acids was removed using a series of organic solvents.

Digital images were acquired using a Gatan 1024 $\times$1024 slow-scan charge coupled device (CCD) camera in a Philips CM-12 TEM operating at 120 kV. We acquired dark field images at the exact two-beam condition for $\mathbf{g}=(220)$ and $\mathbf{g}=(400)$, conditions for which the islands show strong contrast due to strain in the Si substrate.[9] Images (Fig. 1) were acquired with Ge islands on the top (the electron beam entry surface) at a location where the substrate thickness was 550 nm,[10] thick enough to make image contrast relatively insensitive to small changes in thickness or deviation parameter. A thick specimen also reduces to a negligible level the effects of relaxation at the bottom surface. In determining the strain, line profiles parallel to **g** across individual islands were analyzed and compared to simulations. As we will show, the interpretation of image line profiles (Fig. 1) is quite straightforward.

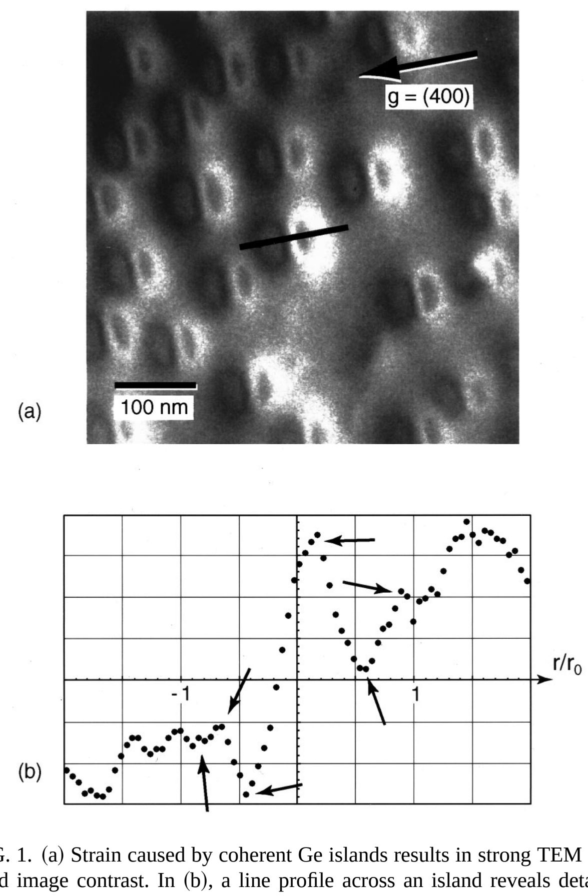


FIG. 1. (a) Strain caused by coherent Ge islands results in strong TEM dark field image contrast. In (b), a line profile across an island reveals detailed structure. Extrema which lie inside the island radius are arrowed.

 

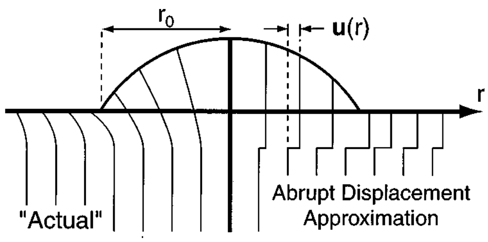


FIG. 2. In the abrupt displacement approximation, the continuous bending of lattice planes is approximated as a step function.

To do this, image simulations were performed by integrating the two-beam Howie–Whelan equations[7,9] using the MATHEMATICA software package. These are a system of coupled first-order ordinary differential equations that can be used to simulate contrast due to strained crystalline specimens if a strain model is available.

Unfortunately, no simple analytical model exists for the strain field due to isolated Ge islands on Si(001). Other researchers have shown that image simulations using finite element (FE) strain fields yield contrast that is qualitatively similar to experimental images,[11,12] however such simulations have not been used for quantitative measurements. It is difficult to measure sample properties such as strain using FE simulations since it is difficult to adjust simulation parameters: one FE simulation is needed to generate each image simulation.

Surprisingly, results can be well explained by using a greatly simplified strain model. We find that when the displacement field decays rapidly compared with the length scale relevant to imaging, i.e., the electron extinction distance (typically ~100 nm), qualitative features can be predicted using a very simple approximation which we call the abrupt displacement approximation (ADA). In this approximation, the continuous displacement field is replaced by a step function a short distance into the substrate (Fig. 2). The size of the step increases linearly from the center to the edge of the island.

In other words, provided that the displacement field decays rapidly enough—within 10–20 nm of the strain source—the ADA allows us to replace any continuous displacement field with a stacking fault-like[9] abrupt displacement which is at a fixed depth and has a variable magnitude. This approximation is useful since TEM image contrast due to stacking faults is well understood. Comparison of this model with image simulations using full strain fields shows that the ADA works well.

Properties of image contrast depend on the scalar product of the diffraction vector used for imaging, **g**, and the displacement field, **u**, via the quantity $\alpha = 2\pi$ **g.u.** If **u** increases linearly parallel to **g**, then $\alpha = 2\pi g(\epsilon r)$, for $r < r_0$ where $r$ is parallel to $g$, $r_0$ is the radius of the island, and $\epsilon = \epsilon_{rr}$, the radial strain in the substrate. Using these assumptions with the ADA, we find that image contrast is periodic with $\alpha$, nearly following a sinusoid. By counting extrema that lie inside the radius of the island the maximum value of the phase $\alpha^{max}$ can be bounded. If $n$ is the number of extrema between the center of the island and the island's edge, then

$$(2n-1)\frac{\pi}{2} < \alpha^{max} < (2n+1)\frac{\pi}{2}.$$

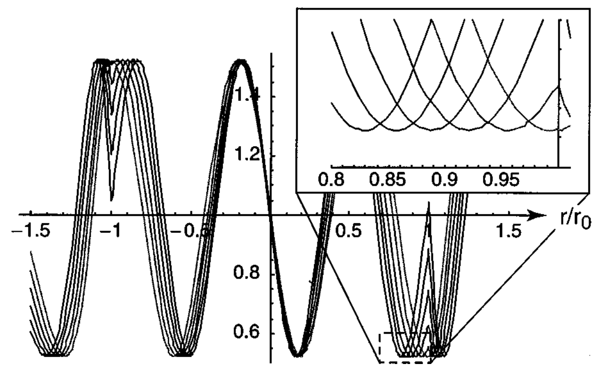


FIG. 3. Simulated image contrast can be used to improve the accuracy of strain measurements. As the slope of $\alpha(r) = \alpha^{max} r/r_0$ increases, the extrema move closer to the center of the island. Here, $\alpha^{max}/(\pi/2)$ varies from 5 (lightest) to 6 (darkest). By analyzing the positions of the extrema in experimental images, accurate strain measurements are possible.

More precise measurements are made by analyzing the positions of intensity extrema inside the island's radius.

Line profiles across islands imaged with a $\mathbf{g} = (400)$ diffraction vector show three extrema, allowing us to place bounds on $\alpha^{max}$. Analyzing the positions of extrema closest to the particle edges improves the measurement. The average position of the outermost extrema for three islands was found to be 0.887 $r_0$, which, when compared with a contrast table (Fig. 3), leads to a value $\alpha^{max}_{(400)} = 8.98\,(=5.72\pi/2)$. By simple algebra, the maximum lattice plane displacement is $\epsilon r_0 = 0.19$ nm and using a weak-beam TEM measurement of the average island radius, we find that $\epsilon = 0.19\,\mathrm{nm}/22.5\,\mathrm{nm} = 0.84 \pm 0.17\%$. We expect that by improving experimental procedures, measurement error less than 10% will be readily achievable.

Our measurement agrees well with FE simulations and with other measurements of the strain. FE results show a maximum displacement $\epsilon r_0 = 0.216$ nm. Converting our strain measurement to a stress (using 170 GPa for the Si Young's modulus and 0.262 for the Poisson ratio), we find $\sigma_{rr} = 1.6$ GPa, a value which lies at the upper end of a recently measured range of stress values for pure Ge on Si(001) during the ''nucleation and growth'' phase of evolution, prior to dislocation introduction.[13] A combined x-ray scanning tunneling microscopy (STM) measurement of strain in an earlier growth phase, when the presence of ''huts'' or ''pyramids'' dominates, led to a strain measurement at the edge of the island equal to 0.5%.[14] Strain has also been measured in islands composed of dilute SiGe alloys on Si(001), and values similar to those measured here have been predicted and measured.[6,15]

We offer the following observations about the measured strain value: first, since the measured maximum displacement matches the results of FE simulations for pure Ge, this suggests that Si has not diffused into the Ge to relax strain. This stands in contrast to electron diffraction strain measurements of pure Ge islands deposited and capped with Si at a much higher temperature (750 °C). In this case the islands were observed to incorporate nearly 40% Si into the Ge.[16]

Second, we note that the maximum displacement of lattice planes, 0.19 nm, is equal to the Burgers vector for an edge dislocation in Si. Displacement of lattice planes greater than this amount would be unlikely since introduction of a dislocation would be energetically more favorable.

In conclusion, we have presented a universal strain measurement technique that does not rely on detailed knowledge of the form of the strain field, and we have used it to measure the in-plane strain in individual coherent Ge islands on Si(001). The measurement agrees well with previous measurements using different techniques, and it suggests that Si diffusion into pure Ge islands does not contribute significantly to stress relaxation in unannealed Ge islands deposited under the present conditions.

*Note added in proof.* While the measurements presented here are correct, subsequent measurements have shown that specimen preparation may affect the strain. We refer the reader to future publications for more extensive measurements of strain in this system.

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