AN ANALYSIS OF GERMANIUM-SILICON/SILICON STRAINED SUPERLATTICE STRUCTURE USING CONVERGENT-BEAM ELECTRON DIFFRACTION

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ABSTRACT

Strained superlattices (SSLs) are typically found inside the p-n junction area of semiconductor devices and consist of very thin alternating layers of different material. There exists a small lattice mismatch between these materials which results in localized strain, as in the case of germanium-silicon/silicon SSLs. Strain measurements using a convergent beam electron diffraction (CBED) technique inside a transmission electron microscope (TEM) have indicated that the strain measured normal to these germanium-silicon/silicon SSLs varies almost sinusoidally, in-spite of theoretical predictions which indicate a much sharper change in strain between these layers. A theoretical formulation involving an elasticity solution has been developed to predict the strain inside these SSL structures. The comparison of theoretical and experimental results clearly quantifies the effect of beam size on the spatial resolution of CBED measurements. Given that beam size is critically dependent on the spot size of the beam, the convergence angle, the specimen thickness, and the position of the focused plane, these parameters are all clearly accounted for in the theoretical predictions.
1. INTRODUCTION

Strained superlattices (SSLs) have become one of the critical elements for building a desirable energy band gap structure at the p-n junction area of semiconductor devices in recent years [1]. The fabrication of SSLs is generally made by means of an epitaxial method [2,3] that allows growth of two types of thin single-crystal layers lattice-matched successively on top of each other. Since the lattice constants of these two types of layers are chosen to be slightly different, the lattice matching causes the layers to be strained elastically. In other words, the accommodation of the lattice mismatch by elastic strain allows each layer to fit to each other without introducing any lattice-mismatch related defects (cf. misfit dislocations) at the interface. The presence of such strain could alter the band structure, for example, in silicon by increasing hole and electron mobility [4], and thus, for the design consideration of functional SSLs, it is essential to understand their microstructural properties, such as the magnitude of mismatch and elastic strain present in the SSL layers. A transmission electron microscope (TEM) is probably the best tool to characterize such properties at a nanometer scale. In the TEM, an electron diffraction technique known as convergent beam electron diffraction (CBED) provides the most sensitive method for determining the magnitude of strain down to the order of $10^{-4}$ on a nano-scale area of the SSL structure. Although the CBED technique has been available for the last two decades, very little work has been done to critically evaluate the importance of its spatial resolution.

In the present work, the CBED technique was employed to critically evaluate the magnitude of elastic strains present in the SSL structure of a TEM specimen. For this, we chose a control sample of SSL that contains well-defined germanium-silicon/silicon (Ge-Si /Si) SSLs.
An elasticity theory that models the strain state of the SSL structure correctly is also formulated to interpret the experimental results. It is shown that the spatial resolution of strain measurements by CBED is affected primarily by the beam size. This finding, assisted by theoretical predictions, is found to be in good agreement with experiments.

2. STRUCTURE OF SSL AND ITS STRAIN RELAXATION OCCURRING IN TEM SAMPLE

The structure of SSLs is typically embedded inside the p-n junction area of semiconductor devices in the form of a finite number of two different alternating layers, each of which is several nanometers thick. There may be lattice mismatch between the two layers that can be accommodated totally by elastic strains, if an appropriate layer thickness/mismatch combination is chosen [2,5]. The elastic strain developed over the layer plane is biaxial in nature, and it induces an additional strain along the direction normal to the layer plane. The introduction of the normal strain results from the so-called “tetragonal distortion” phenomenon [6].

Fig. 1. (a) A schematic picture of a bulk material containing 5 layers of A/B superlattice and (b) a thin (100 ~400 nm) slice of TEM specimen taken out of the bulk specimen.

Figure 1(a) is a schematic view showing 5 A/B alternating layers of SSL sandwiched between two semi-infinite media A. In this bulk structure, only the B layers are strained, because the SSL is surrounded by two semi-infinite A materials. Namely, the B layer is subjected to a biaxial strain over the y-z plane and the associated normal strain by tetragonal
distortion. Thus the geometry shown in Fig. 1(a) is considered to represent a bulk form of the SSL structure. For a TEM analysis of this SSL structure, a thin slice is taken out of the bulk, as seen in Fig. 1(b). Then it is clear that the whole strain pattern inside the TEM specimen will be altered according to the magnitude of the mismatch, the layer thickness, and the specimen thickness. A cross-sectional view of this strain relaxation can be further clarified in Fig. 2, where it is illustrated schematically how the two-dimensional square elements of A and B lattices, whose bulk lattice constants are $a_A$ and $a_B$ ($a_A < a_B$), will deform inside the TEM specimen configuration. In this thin film case, it is easy to see that the presence of the top and bottom surfaces modify the strain pattern of the bulk (cf. Fig. 2(b)). For this reason, the strain change can also be termed “surface relaxation”.

*Fig. 2. A schematic illustration showing how (a) the B layer of a thin specimen containing five A/B strained superlattice layers in the A matrix undergoes (b) an elastic relaxation. The shape change in the grid pattern indicates the relaxation. The lattice constants of square cells for A and B are designated as $a_A$ and $a_B$. The thickness of the specimen is $t$.*

Germanium-silicon (Ge-Si) alloy and silicon (Si) can be used as an example of the SSL described above. Namely, Si and Ge-Si materials represent A and B media exemplified in Figs. 1 and 2. Germanium and silicon, both diamond cubic, are convenient semiconductor materials for producing the SSLs, because they form a solid solution alloy over the entire composition range. Thus the lattice constant of the alloy can be easily varied by changing the Ge-to-Si ratio and its magnitude can be estimated using an empirical relationship [7];

*In analogy to the terminology used for fabricating the hetero-structure of III-V compound semiconductors, the layers Ge-Si and Si can be referred as quantum well (QW) and barrier layers, respectively.*
where \( a_{Ge,Si_{1-x}} \) is the lattice constant of the \( Ge_xSi_{1-x} \) alloy and \( x \) is the atomic concentration of Ge. Then the amount of the lattice misfit between \( Ge_xSi_{1-x} \) and Si can be defined as

\[
\frac{a_{Ge,Si_{1-x}} - a_{Si}}{a_{Si}} = f \left( a_{Ge,Si_{1-x}} > a_{Si} \right)
\]

where \( a_{si} \) is the lattice constant of Si.

Equations (1) and (2) are used in the subsequent elasticity theory.

3. ELASTICITY SOLUTION OF SSL

Fig. 3. x-y coordinate and geometrical parameters used for computing strains in the Ge-Si/Si layers. The layer thicknesses of Ge-Si and Si are \( d_1 \) and \( d_2 \), respectively, whereas the film thickness is \( t \).

An analytical solution applicable to the SSL configuration in Fig. 2 can be obtained using the Fourier series method. Such a formulation was first given by Treacy and Gibson [8 - 10], who obtained isotropic and anisotropic elasticity solutions on the basis of Timoshenko and Goodier’s classical beam theory [11]. A similar formulation specific to the geometry corresponding to the present experiment is used for this analysis. In Fig. 3, the x-y coordinate system for the cross-sectional view of 5 Ge-Si QW layers sandwiched by Si buffer layers is illustrated. This section is bounded by two semi-infinite Si media. To distinguish the location of the QWs, they are marked with symbols as follows: QW#1, QW#2, QW#3, QW#4, and QW#5.
From the present formulation, the detail of which will be published subsequently, the normal strain, \( \varepsilon_{xx} \), along the \( x \) direction is obtained. The bar sign over the strain, \( \bar{\varepsilon}_{xx} \), indicates that the strain is averaged over the specimen thickness \( t \), which is directly comparable with experimental strain values obtained by the CBED technique. Then \( \bar{\varepsilon}_{xx} \) can be expressed as

\[
\bar{\varepsilon}_{xx}(x) = \frac{5}{2} \left( 1 - \nu \right) \left( 1 + \frac{f}{1 - \nu} \right) \left( \frac{d_1}{l} \right) \\
+ \left( 1 + \frac{f}{1 - \nu} \right) \left( \frac{2}{l} \right) \sum_{m=1}^{\infty} \frac{\sin(\alpha_m d_1 / 2)}{\alpha_m} \left\{ 1 + 2 \cos(\alpha_m d) + 2 \cos(2\alpha_m d) \right\} \times (3)
\]

\[
\times \left[ 1 - 8 \nu \sinh^2(\alpha_m t / 2) \left( \frac{\alpha_m t}{(\alpha_m t + \alpha_m t)} \right) \cos(\alpha_m x) \right]
\]

where \( f \) is the amount of misfit between the Si and Ge-Si, \( l \left( >> 2 \frac{1}{2} d_1 + 2 d_2 \right) \) an arbitrary constant, and \( \alpha_m = \frac{m\pi}{l} \ (m = 1, 2, 3 \cdots n) \). In this formulation, it is assumed that the Poisson’s ratio, \( \nu \), of both the Si and Ge-Si alloy is identical. The magnitude of \( \bar{\varepsilon}_{xx} \) was determined experimentally and compared with the theoretical value of Eq. (3).

4. EXPERIMENTAL

The SSL specimen used in this study was a commercially-available TEM sample for thickness calibration, known as “Magical™”. This specimen comes as the \{110\} cross section sample and contains the SSL structure that consists of 5 alternating layers of Si and Ge-Si alloy with a specific layer thickness and composition, which were grown epitaxially on \{001\} silicon substrates. This SSL geometry is the same as that shown in Figs. 1, 2, and 3. For the CBED analysis, the [340] zone was chosen, because it provides good visibility of
high-order-Laue-zone (HOLZ) lines. Another advantage of using this particular zone was that only a small tilt angle of 8° is required to reach the zone from the (110) cross-section while keeping the (001) plane parallel to the beam direction.

CBED HOLZ patterns were obtained in a scanning (STEM) mode using a JEOL 2100 field-emission TEM operated at an accelerating voltage of 200 kV. From the full width at half maximum of the probe’s intensity profile, the focused probe size (in diameter) was determined to be ~1.03 nm. The half convergence angle of the probe was ~14.3 mrad and CBED patterns were recorded using a Gatan’s Ultrascan 2k×2k pixel CCD camera. Further details of the experimental CBED measurements can be found in Dr. Mogili’s PhD thesis [12].

Java Electron Microscope Simulation (JEMS®) software [13] was used to simulate HOLZ lines both kinematically and dynamically in the Bloch-wave formalism. The simulated HOLZ patterns were first employed for the purpose of calibrating both the camera constant and the accelerating voltage of the TEM, which was found to be 202.10 kV. Then the magnitude of strains was determined by comparing experimental HOLZ patterns with simulations.

5. RESULTS AND DISCUSSION

In the (110) cross-section of the SSL specimen, the two principal strains, $\varepsilon_{xx}$ and $\varepsilon_{yy}$, were available for CBED measurements. Only the former strain change, however, was large enough to yield a measurable quantity. Consequently, only the normal strain ($\varepsilon_{xx}$) is presented around QW#1 (see Fig. 3). Figure 4 shows experimental and theoretical plots of
\( \varepsilon_{xx} \) measured around the QW #1 at the specimen thickness, \( t \), of 258 nm. For the theoretical plot, Equation (3) is used, for which \( d_1(=d_2)=12 \text{ nm} \), \( \nu=0.25 \), and \( f=0.008 \). In terms of atomic concentration \( x \) of Ge (\( \text{Ge}_x\text{Si}_{1-x} \)), the magnitude of this misfit correspond to \( x=0.21 \) (see Eq. (1)). Similar plots for a thicker \( (t=474 \text{ nm}) \) specimen are shown in Fig. 5. For both the thicknesses, the shape of the experimental curves for \( \varepsilon_{xx} \) is characterized as consisting of a top flat (TF) region surrounded by the symmetrical left/right shoulders (S) with a linear slope. In contrast to the experimental curves, the corresponding theoretical curves are almost a square step, containing only the TF region without the sloped S region. Apparently, there is a large discrepancy in the size of the S and TF regions between the experiments and the theoretical predictions.

The origin of the linear slope, S, in the experimental plots was further investigated. It was thought that the linear slope, S, could originate from two possible sources; (1) there is an interdiffused region between the Ge-Si and Si layers, or (2) the beam size is large due to beam broadening. These two possible sources were analyzed more in detail in the following sections.

**Fig. 4.** Strain \( \varepsilon_{xx} \) averaged over the specimen thickness \( (t=258 \text{ nm}) \) plotted against the lateral distance \( x \). Both experimental and theoretical results are plotted.

**Fig. 5.** Strain \( \varepsilon_{xx} \) averaged over the specimen thickness \( (t=474 \text{ nm}) \) plotted against the lateral distance \( x \). Both experimental and theoretical results are plotted.

5.1. Possible presence of interdiffused region between Ge-Si and Si
As a cause for the linearly-sloped shoulders in the experimental $\varepsilon_{xx}$, the possibility that the Ge-Si QW layers could be interdiffused with the neighboring Si buffer layers was first considered. The most direct method for detecting the presence of such an interdiffused layer is to use a high-angle-annular-dark-field (HAADF) imaging method that provides image contrast variations sensitive to the atomic number; the Ge-Si QW layer containing Ge atoms with a high atomic number should show up as a brighter band. Figure 6 is the image of HAADF taken from 5 QW/buffer SSL layers, which are sandwiched between Si. The QW layers are seen as 5 white stripes in the dark background, which consists of Si. This well-defined image of white band clearly indicates that there is no contrast gradient in the Ge-Si/Si interfacial region, indicative of possible interdiffusion. Thus the presence of an interdiffused region between the QW and buffer layers was ruled out. It should be noted that there is a fine periodic contrast change inside the QW region (seen as two or three grey lines) inside the five white bands. These fine gray-colored periodic lines represent compositional modulation in the Ge and Si ratio; these lines are actually Ge-deficient region induced by the substrate rotation during the film growth [14,15]. This type of compositional change, however, is usually small. In fact this modulation does not contribute to variations in the $\varepsilon_{xx}$ curves. Thus this small compositional modulation does not conflict with the conclusion that there is no interdiffusion between the QW and its neighboring buffer layers.

Fig. 6. A HAADF image taken from strained Ge-Si/Si superlattice layers, containing 5 layers (seen as white) of Ge-Si in the matrix of Si (dark area) (Courtesy of Dr. Dong Tang, FEI Inc., August 2008).
5.2 Beam broadening

Based on the HAAF imaging result, the possibility of interdiffusion inside the SSL was ruled out. The only other possible cause for the discrepancy observed in the $\tilde{\varepsilon}_{xx}$ curve between the experiment and the theory is considered to be due to beam broadening, which can be described in terms of the beam size. Unlike the spot size, the beam size defined here is not a stationary value, but changes with experimental conditions. The detail of the difference between the two terminologies, i.e. spot size and beam size, will be described in the following section. The main idea here is to estimate the effect of the beam size on $\tilde{\varepsilon}_{xx}$ theoretically and then compare it with the experiment. The effect of the beam size can be easily incorporated into the theory. Assume that the beam size (in diameter) is $\delta$, and then the beam size dependent strain, $\varepsilon^{BS}_{xx}$, can be expressed by integrating Eq. (3) from $x-\delta/2$ to $x+\delta/2$ and then by averaging over $\delta$, i.e.

$$
\varepsilon^{BS}_{xx} = \int_{x-\delta/2}^{x+\delta/2} \varepsilon_{xx} dx \over \delta
$$

(4)

where the superscript, BS, in $\varepsilon^{BS}_{xx}$ indicates that the effect of the beam size on $\tilde{\varepsilon}_{xx}$ is taken into account. In this formulation, it is assumed that each beam spot creates a $t$-long cylinder whose diameter is $\delta$. In the present case, the geometry is one-dimensional, so the beam spot produces a rectangle with the width of $\delta$ and the length of $t$. Substitution of Eq. (3) into Eq. (4) yields
\[- \frac{\varepsilon_{xx}}{\varepsilon_{xx}^{BS}} = \frac{5}{2} (1-\nu) \left( \frac{1+\nu}{1-\nu} f \right) \left( \frac{d_i}{l} \right) + \left( \frac{1+\nu}{1-\nu} f \right) \left( \frac{2}{l} \right) \left( \frac{1}{\delta} \right) \sum_{m=1}^{\infty} \sin \left( \frac{\alpha_m d_i}{2} \right) \left\{ 1 + 2 \cos \left( \alpha_m d_i \right) + 2 \cos \left( 2 \alpha_m d_i \right) \right\} \times \left[ 1 - 4\nu \frac{\{ 1 - 2e^{-\alpha_m t} + e^{-2\alpha_m t} \}}{\{ 1 - e^{-2\alpha_m t} + 2(\alpha_m t)e^{-\alpha_m t} \}} \right] \left[ \sin \left\{ \alpha_m \left( x + \delta / 2 \right) \right\} - \sin \left\{ \alpha_m \left( x - \delta / 2 \right) \right\} \right] \right\}

(5)

To see how the beam size affects the $\varepsilon_{xx}$ theoretically, a composite map is made of $\varepsilon_{xx}^{BS}$ as a function of the beam size, $\delta$ using Eq. (5). Figure 7 is the map for the 258 nm thick specimen. If the effect of the beam size is taken into account, the shoulder region appears in the theoretical curves. One consistent trend in this map is that the shoulder slope is always linear regardless of the magnitude of the beam size, while its absolute value decreases and, at the same time, the top flat region shrinks with increasing beam size. Since the shoulder slope of the experimental curve seen in Fig. 4 is roughly linear, they are directly comparable with the theoretical curves, if an appropriate beam size is selected. Similar trend was observed for the 474 nm thick specimen. These theoretical predictions strongly suggest that the beam size is a primary factor for affecting the shape of the experimental $\varepsilon_{xx}$ curves.

Fig. 7. A theoretical composite map showing the effect of beam size $\delta$ on the average strain $\varepsilon_{xx}^{BS}$ for the SSL specimen of thickness $t = 258$ nm.

5.3 Estimate of the beam size using the slope of shoulders
A more accurate assessment of the experimental $\tilde{\varepsilon}_{xx}$ with respect to the theoretical prediction can be completed quantitatively by comparing the value of the shoulder slope. For this comparison, Equation (5) is differentiated with respect to $x$, yielding the slope of $-\frac{\partial \tilde{E}_{xx}}{\partial x}$ as

$$
\frac{\partial \tilde{E}_{xx}}{\partial x} = -(1 + \nu f) \frac{2}{l} \frac{2}{d} \sum_{m=1}^{\infty} \frac{\sin(\alpha_m d/2)}{\alpha_m} \left\{1 + 2 \cos(\alpha_m d) + 2 \cos(2\alpha_m d)\right\} \times
$$

$$
\left[1 - 4\nu \left\{\frac{1 - 2e^{-\alpha_m t} + e^{-2\alpha_m t}}{\alpha_m t}\right\}\left\{1 - e^{-2\alpha_m t} + 2(\alpha_m t)e^{-\alpha_m t}\right\}\right] \sin\left(\alpha_m \delta / 2\right) \sin(\alpha_m x)
$$

(6)

The average experimental slope for $t = 258 \text{ nm}$ was found to vary from $1.4 \times 10^{-3}$ to $1.7 \times 10^{-3} \text{ nm}^{-1}$, whereas that for $t = 474 \text{ nm}$ changed between $1.5 \times 10^{-3}$ and $1.7 \times 10^{-3} \text{ nm}^{-1}$.

Figures 8 and 9 are the plots of $-\frac{\partial \tilde{E}_{xx}}{\partial x}$ evaluated at $x = -54 \text{ nm}$. Intersections with the grey band indicates the upper and lower limits of the experimental slopes, give the beam size to lie between 7.4 and 8.4 nm for $t = 258 \text{ nm}$, whereas, they range from 7.9 to 8.8 nm for $t = 474 \text{ nm}$. The range of the beam size for $t = 258 \text{ nm}$ appears to be slightly smaller than that for $t = 474 \text{ nm}$. Since the difference is small, it is considered that the beam size is similar for both thicknesses.

**Fig. 9. The slope of the shoulder, $-\frac{\partial \tilde{E}_{xx}}{\partial x}$, plotted as a function of beam size $\delta$ for the specimen thickness of 258 nm using Eq. (6). Experimental slope values lie within the shaded band. The intersection of the band with the theoretical curve reflects the possible range of the beam size, which was $\delta = 7.4 \sim 8.4 \text{ nm}$.**
Fig. 10. The slope of the shoulder, \( \frac{\partial \varepsilon_{xx}}{\partial x} \bigg|_{x=-54} \), plotted as a function of beam size \( \delta \) for the specimen thickness of 474 nm using Eq. (6). Experimental slope values lie within the shaded band. The intersection of the band with the theoretical curve yields the possible range of the beam size, which was \( \delta = 7.9 \sim 8.8 \) nm.

Fig. 11. Comparison of experimental \( \bar{\varepsilon}_{xx} \) with the corresponding theoretical result that takes the beam size into account. The beam size \( \delta \) is 8 nm.

Fig. 12. Comparison of experimental \( \bar{\varepsilon}_{xx} \) with the corresponding theoretical result that takes the beam size into account. The beam size \( \delta \) is 8 nm.

Based on the above results using the shoulder slope comparison, it is concluded that the average beam size is 8 nm for both thicknesses. Accordingly, the theoretical curves are plotted on top of the experimental ones in Figs. 10 and 11. Although the overall curve matching is not perfect, it is acceptable because of experimental uncertainties.

5.4 Estimate of the beam size using the geometry of beam propagation

It has been shown in the previous section that the shoulder slope can be used as an estimate of the beam size. The validity of such a method can be further tested from the simple geometrical analysis of beam propagation. The geometrical analysis is described in the following.

In this paper, the focused spot formed by a convergent (non-parallel) beam on the specimen will be referred as the spot size (in diameter), \( \delta_{SS} \). While the beam propagates down the specimen, such a spot can be broadened according to the convergence angle
and the distance it travels. In other words, the diameter of the spot increases as the beam travels down the specimen. The increased spot size projected along the thickness direction onto the bottom surface of the specimen will be defined as “beam size”. It is thus easy to understand that the beam size is not a stationary value but changes with the film thickness, the angle of beam convergence, and the location of focus. Following Ruh’s description [16], two limiting cases are illustrated in Fig. 12, in which the convergent beam is focused (a) at the top surface and (b) at the middle plane. These two cases represent the occurrence of the maximum beam size of $\delta_{\max}$ (Case (a)) and the minimum beam size of $\delta_{\min}$ (Case (b)). Accordingly, the beam size, $\delta$, is a function of the spot size, the specimen thickness, and the location of the focal plane. The beam size changes from the minimum value of $\delta_{\min}$ to the maximum value of $\delta_{\max}$, i.e. $\delta_{\min} \leq \delta \leq \delta_{\max}$. It should be noted that the above assumption is true as long as the convergent beam travels normal to the wavefront without bending and the focus plane lies between the top and bottom surfaces. In other words, no over- or under-focusing outside the specimen is allowed. Now it is easy to show the following two relationships [7] from Fig. 12.

$$\delta_{\min} = \delta_{SS} + \alpha_c t$$  \hspace{1cm} (7)

$$\delta_{\max} = \delta_{SS} + 2\alpha_c t$$  \hspace{1cm} (8)

where $\delta_{SS}$ is the spot size, $\alpha_c$ the half convergence angle, and $t$ the specimen thickness.

The maximum and minimum values of the beam size, i.e. $\delta_{\max}$ and $\delta_{\min}$, can be calculated from Eqs. (7) and (8). This result is listed in Table 1. For the thickness of 258 nm, the beam size varies from 4.7 to 8.4 nm, whereas, for the 474 nm thick specimen, it changes from 7.8 to 14.6 nm. It is surprising to note that the theoretical predictions obtained by
the shoulder slope method come within the range of the beam size estimated by the geometrical analysis. This confirms the validity of using the shoulder slope for comparison. Again, considering the fact that there is an uncertainty in the exact focus plane, the experiment appears to be in good agreement with the theory.

*Fig. 12.* A schematic illustration showing how the beam size changes during the propagation of the convergent beam inside the specimen. (a) The beam is focused at the top surface and (b) at the middle plane. \( \delta \) is the final beam size at the bottom (exit) surface, \( \alpha_c \) is the half convergence angle, \( \delta_{ss} \) the spot size, and \( t \) the film thickness.

*Table. 1.* The computed values of \( \delta_{\text{min}} \) and \( \delta_{\text{max}} \) for \( t = 258 \) and 474 nm using Eqs. [A-1] and [A-2] in Appendix A. Note that \( \alpha_c = 14.33 \text{ mrad} \) and \( \delta_{ss} = 1.03 \text{ nm} \).

<table>
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<th>Thickness (nm)</th>
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<td>8.4</td>
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<tr>
<td>474</td>
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5.5 Spatial resolution of strain measurements by CBED

The spatial resolution of strain measurements by the CBED technique can be defined as a minimum distance between two beam spots that provide independent strain values without any interference. In practice, the beam broadening causes each spot to generate a cylindrical volume. When two cylinders defined by two beam spots come into contact, the center-to-center distance of the two cylinders becomes the smallest distance, which is
exactly the beam size. Consequently, the beam size becomes the spatial resolution. In the present strain measurements, the spatial resolution is ~8 nm, which is the average beam size.

With the spatial resolution of ~8 nm, it is important to answer why the experimental curves exhibited the sloped shoulder. One of the reasons is that the lateral feature size of each layer (~12 nm) was very close to the beam size (or the spatial resolution) (~8 nm), making the overlapping of strains from the neighboring features inevitable. In the present SSL configuration, therefore, the magnitude of lateral feature size appears to become a limiting factor for strain measurements by CBED. Nevertheless, the spatial resolution can be improved if one uses a thinner specimen or a specimen containing a feature size larger than the beam size.

6. CONCLUDING REMARKS

A CBED technique was used to analyze the distribution of the principal strain induced by the tetragonal distortion, which is developed inside the germanium-silicon/silicon SSL layers. Based on the geometry of the SSL, an elasticity theory was formulated and used to compare with the experiment. It was found that there is a large discrepancy between the experiments and the theoretical predictions. If the effect of the beam size is considered, it is possible to match the theoretical strain curve to the experimental one; the experimental curves can be explained by considering the effect of the beam size. The origin of the discrepancy between the experiment and the theoretical predictions was found to be the beam size, which is the spatial resolution of the CBED strain measurements. The beam size depends critically on the spot size of the beam, the convergence angle, the specimen thickness, and the position of the
focused plane. Experimental strain results were found to be in qualitative agreement with theoretical predictions, if the beam size in the order of ~8 nm in diameter was assumed. Finally, although the elasticity theory takes the surface into account, the effect of surface relaxation did not affect the overall strain distribution due to the relatively thick (258 and 474 nm) specimens used.
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Fig. 6. A HAADF image taken from strained Ge-Si/Si superlattice layers, containing 5 layers (seen as white) of Ge-Si in the matrix of Si (dark area) (Courtesy of Dr. Dong Tang, FEI Inc., August 2008).
Fig. 7. A theoretical composite map showing the effect of beam size $\delta$ on the average strain $\varepsilon_{xx}^{BS}$ for the SSL specimen of thickness $t = 258 \text{ nm}$. 
Fig. 8. The slope of the shoulder, \( \frac{\partial E_{ss}}{\partial x} \bigg|_{x=-54} \), plotted as a function of beam size \( \delta \) for the specimen thickness of 258 nm using Eq. [6]. Experimental slope values lie within the shaded band. The intersection of the band with the theoretical curve reflects the possible range of the beam size, which was \( \delta = 7.4 \sim 8.4 \text{ nm} \).
Fig. 9. The slope of the shoulder, \( \frac{\partial E_{ss}}{\partial x} \bigg|_{x=-54} \), plotted as a function of beam size \( \delta \) for the specimen thickness of 474 nm using Eq. [6]. Experimental slope values lie within the shaded band. The intersection of the band with the theoretical curve yields the possible range of the beam size, which was \( \delta = 7.9 \sim 8.8 \text{ nm} \).
Fig. 10. Comparison of experimental $\varepsilon_{xx}$ with the corresponding theoretical result that takes the beam size into account. The beam size $\delta$ is 8 nm.
Fig. 11. Comparison of experimental $\tilde{\varepsilon}_{xx}$ with the corresponding theoretical result that takes the beam size into account. The beam size $\delta$ is 8 nm.
Fig. 12. A schematic illustration showing how the beam size changes during the propagation of the convergent beam inside the specimen. (a) The beam is focused at the top surface and (b) at the middle plane. $\delta$ is the final beam size at the bottom (exit) surface, $\alpha_c$ the half convergence angle, $\delta_{ss}$ the spot size, and $t$ the film thickness.