Depth profiles of the interfacial strains of Si$_{0.7}$Ge$_{0.3}$/Si using three-beam Bragg-surface diffraction

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Interfacial strains are important factors affecting the structural and physical properties of crystalline multilayers and heterojunctions, and the performance of the devices made of multilayers used, for example, in nanowires, optoelectronic components, and many other applications. Currently existing strain measurement methods, such as grazing incidence X-ray diffraction (GIXD), cross-section transmission electron microscopy, TEM, and coherent diffractive imaging, CDI, are limited by either the nanometer spatial resolution, penetration depth, or a destructive nature. Here we report a new non-destructive method of direct mapping the interfacial strain of [001] Si$_{0.7}$Ge$_{0.3}$/Si along the depth up to ~287 nm below the interface using three-beam Bragg-surface X-ray diffraction (BSD), where one wide-angle symmetric Bragg reflection and a surface reflection are simultaneously involved. Our method combining with the dynamical diffraction theory simulation can uniquely provide unit cell dimensions layer by layer, and is applicable to thicker samples.

Bragg-surface diffraction (BSD)$^{1-4}$ occurs when the sample crystal is first aligned for a symmetric Bragg reflection, say G, by adjusting the Bragg angle $\theta_B$ and then the crystal is rotated by the azimuth, $\phi$, around the reciprocal lattice vector $\mathbf{g}$ of the G-reflection, without disturbing the G reflection, to bring an additional surface reflection, L, also satisfying Bragg’s law (Fig. 1a). In reciprocal space (Fig. 1b), three reciprocal lattice points (r.l.p.), O, G, and L, are moved onto the surface of the Ewald sphere. Thus three r.l.p., O, G, and L, lie simultaneously on the surface of the Ewald sphere and excite three beams along the wavevectors, $\mathbf{K}_O$, $\mathbf{K}_G$, and $\mathbf{K}_L$. Three-beam BSD thus occurs$^5$. For clarity, (G/L) is used to denote the three-beam BSD. Since point L is on the equatorial plane, the reflected beam is propagating along the crystal surface, thus the grazing-exit diffraction, L, provides scattering information from the surface, interface, up to the depth comparable with the extreme depth limitation by the evanescent waves of the Bragg reflection G. The geometries of the real and reciprocal space are shown in Fig. 1a,b, respectively.

The heterojunction$^{6-9}$, Si$_{0.7}$Ge$_{0.3}$/Si, is prepared by using a germanium silicide target to grow a thin-film of Si$_{0.7}$Ge$_{0.3}$ on silicon substrate by molecular beam epitaxy, MBE, in National Nano Device Laboratory, NDL. In addition, before the epitaxial process, the Si wafer clearance is a standard manufacturing procedure, i.e., the surface particles and native SiO$_2$ are removed. An energy dispersive spectrum, EDS, is employed to measure compositions versus depth (Si ~0.7 ± 0.01 and Ge ~0.3 ± 0.01, see Fig. 2d). The 0–20 scans, namely q-scans, of the conventional X-ray Bragg diffractions (shown in Fig. 2a–c) from 400, 040 and 004 reflections at 12 keV reveal that the a- and b-axis of the two materials, Si$_{0.7}$Ge$_{0.3}$ and silicon, are very close to each other. By the modelling data (solid line in red) of Fig. 2a–c, the a- and b-axis are about 5.428 and 5.4256 Å, respectively, in the Si$_{0.7}$Ge$_{0.3}$ thickness, $d_{SiGe}$ (~57 nm). The c-axes of the Si$_{0.7}$Ge$_{0.3}$ and silicon substrate are about 5.5344 and 5.4345 Å, because of two distinct 004 peaks (Fig. 2c). In such an epitaxial process, the most stable heterostructure occurs when the a- and b-axis of the Si$_{0.7}$Ge$_{0.3}$ are compressed to match that of the Si substrate, along with the stretched c-axis of the Si$_{0.7}$Ge$_{0.3}$. Here, referring to the measured bulk value, 5.4898 Å, of Si$_{0.7}$Ge$_{0.3}$, the tensile strains along the a-, b-, and c-axis are about $-0.011$, $-0.011$ and 0.008, respectively. Furthermore, the epitaxial process not only caused the tensile strains but also shear strains, thus the lattice parameters under study are assumed to have the degrees of freedom along the tensile and shear directions. To confirm the lateral distribution of the thin-film system, the X-ray reflectivity, XRR, is adopted to measure the thickness of Si$_{0.7}$Ge$_{0.3}$ and the roughnesses of the surface and interface of the Si$_{0.7}$Ge$_{0.3}$/Si. The experiment and simulation of the XRR data (see ref. 10) are shown in Fig. 2e.

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The azimuth rotation, \( \phi \), is reflected by the sample at the Bragg angle, \( \theta_B \), which is parallel to the surface. The three lattice unit vectors, \( \hat{a}, \hat{b}, \hat{c} \), of the \( \text{Si}_{0.7}\text{Ge}_{0.3} \) unit cell are estimated by matching the measured and the calculated intensity distributions, for both tth- and beta-scans. The combined boundary conditions of EM fields, covering each atomic layer along \([001]\), are considered in the calculations based on the dynamical theory of X-ray diffraction for layered crystalline material\(^{11,12}\). For an X-ray penetration depth about 287 nm (see Supplementary Figure 5), 1000 atomic layers of about 5.43 Å thick each are considered. Since the same 004 reflection is involved in the three sets BSD's, the three lattice unit vectors can be uniquely determined along the depth\(^{13}\).

The BSD diffraction experiments of \( \text{Si}_{0.7}\text{Ge}_{0.3} / \text{Si} \) are carried out at beamline 17B1, Taiwan Light Source (TLS), National Synchrotron Radiation Research Center (NSRRC). For the BSD, 004/202, 004/022 and 004/422, for \( \text{Si}_{0.7}\text{Ge}_{0.3} \) and three surface reflections, 202, 022 and 422, for Si substrate are measured along the vertical two theta (tth) and horizontal (beta) scans of the surface diffracted beams (Fig. 2a). The 004 is a wide-angle symmetric reflection, which ensures large penetration in the crystal due to the large incidence angle. The three lattice unit vectors, \( \hat{a}, \hat{b}, \hat{c} \) of \( \text{Si}_{0.7}\text{Ge}_{0.3} \) and Si unit cells are estimated by matching the measured and the calculated intensity distributions, for both tth- and beta-scans. The combined boundary conditions of EM fields, covering each atomic layer along \([001]\), are considered in the calculations based on the dynamical theory of X-ray diffraction for layered crystalline material\(^{11,12}\). For an X-ray penetration depth about 287 nm (see Supplementary Figure 5), 1000 atomic layers of about 5.43 Å thick each are considered. Since the same 004 reflection is involved in the three sets BSD's, the three lattice unit vectors can be uniquely determined along the depth\(^{13}\).

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The BSD in reciprocal space: the \( \phi \) rotation brings an additional reciprocal lattice point, \( L \), onto the surface of the Ewald sphere in the equatorial plane, thus three reciprocal lattice points, \( O, G, L \) being on the surface of the Ewald sphere simultaneously.

From the simulation, the \( \text{Si}_{0.7}\text{Ge}_{0.3} \) thickness, \( d_{\text{SiGe}} \), is about 58.5 nm. The roughnesses of the surface (\( \sigma_{\text{surface}} \)) and interface (\( \sigma_{\text{interface}} \)) are about 0.9 and 1.1 nm, respectively. Moreover, through the image of high-resolution transmission electron microscope, HRTEM, the local probe of the \( \text{Si}_{0.7}\text{Ge}_{0.3} \) thickness is about 59.9 nm (Fig. 2f), and the interfacial lattice array is also shown in Fig. 2g.

Due to the structural proximity of the \( \text{Si}_{0.7}\text{Ge}_{0.3} \) film and the Si substrate, three sets of three-beam BSD, 004/202, 004/022 and 004/422, for \( \text{Si}_{0.7}\text{Ge}_{0.3} \) and three surface reflections, 202, 022 and 422, for Si substrate are measured along the vertical two theta (tth) and horizontal (beta) scans of the surface diffracted beams (Fig. 2a).

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Figure 3a shows schematically the tth- and beta-scans of the 202 surface diffraction. For the tth-scan, the two peaks p1 and p4 are the 202 surface diffractions from \( \text{Si}_{0.7}\text{Ge}_{0.3} \) and Si respectively. The other two peaks, p2, p3, respectively.

The simulations are started from finding unique solutions for the three lattice unit vectors, \( \hat{a}, \hat{b}, \hat{c} \), of the \( \text{Si}_{0.7}\text{Ge}_{0.3} \) thin-film and silicon substrate so that the simulated intensity distributions fit the measured ones. Namely, the elements of the metric tensor, \( \sigma \), defined below will be determined,

\[
\sigma = \begin{bmatrix}
\sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\
\sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\
\sigma_{zx} & \sigma_{zy} & \sigma_{zz}
\end{bmatrix}
\]

where \( \sigma = (a_x, a_y, a_z) \), \( b = (b_x, b_y, b_z) \) and \( c = (c_x, c_y, c_z) \). The peak positions of the tth- and beta-scans of the three surface reflections, 202, 022 and 422 given above are used to solve the tensor \( \sigma \).
According to Supplement Ι, the measured θ and β of p1 from the three surface diffractions (Figs 3b–f and 4 and Supplementary Figure 8) give the nine elements of the Si0.7Ge0.3, denoted as σ₁. Similarly, the measured θ and β of p4 from Figs 2 and 3 determine the nine elements of the Si substrate as σ₂. For clarity, the tensor elements of σ₁ are labeled as (ax₁, ay₁, az₁), (bx₁, by₁, bz₁), (cx₁, cy₁, cz₁) and that of σ₂ as (ax₂, ay₂, az₂), (bx₂, by₂, bz₂), (cx₂, cy₂, cz₂).

As the samples are high-quality crystals with narrow peak widths (Fig. 2c), the dynamical theory of X-ray diffraction3,11,12,15 is employed in the simulations. The interface of Si0.7Ge0.3/Si is usually very sharp, however, in terms of an Angstrom scale, the interface can be treated as a gradual change from the Si0.7Ge0.3 thin-film to silicon substrate. Furthermore, with the EDS data (Fig. 2e) and Vegard’s law, the predictions of the lattice parameter vs. depth follow approximately the Boltzmann function (see Supplementary Figure 4). Namely, the nine elements of the tensor σ₁ for each atomic layer can be determined from the σ₁ (Si0.7Ge0.3) and σ₂ (Si) at corresponding depth, x, using the Boltzmann function as an approximation:

\[
B(x) = \frac{\text{lat}_1 - \text{lat}_2}{1 - e^{-\frac{x-x_0}{\text{lat}_2 - \text{lat}_1}}},
\]

where the symbol, x, is the depth from the crystal surface, and x₀ is the thickness of the Si0.7Ge0.3, determined from the Bragg peak at p1. The two constants, lat₁ and lat₂, are the corresponding elements of the tensors, σ₁ and σ₂.
Figure 3. The experiment of Bragg-surface diffraction. (a) In the laboratory coordinate, the forward diffracted beam, $\vec{K}_O$, is along the positive x-axis, and is diffracted into $\vec{K}_G$ and $\vec{K}_L$ directions. The intensity of the surface diffraction along $\vec{K}_L$ is measured by a $\theta$-scan perpendicular and a $\beta$-scan parallel to the x-y plane of the laboratory coordinate. Peaks, p1 and p4 are the surface diffraction from the thin-film, Si$_{0.7}$Ge$_{0.3}$, and the silicon substrate. Peaks p2 and p3 and the undulating background are the Si$_{0.7}$Ge$_{0.3}$ Kiessig fringes. The slit widths of the vertical $\theta$-scan and horizontal $\beta$-scan are about 10 $\times$ 0.1 and 0.1 $\times$ 0.1 mm (H $\times$ V). (b) The measured (red square dot) and simulated (black solid line) $\theta$-scan of the surface diffraction, 202 of the BSD, 004/202, shows the two diffracted peaks, p1 and p4, and the Kiessig fringes including p2 and p3. The top and bottom abscissas are $\theta$ (in deg.) and the corresponding z-component, $q_z$ (in Å$^{-1}$), of the scattering vector, $\vec{q}$ (where $\vec{q}$ = ($q_x$, $q_y$, $q_z$) = $\vec{K}_L$ $-$ $\vec{K}_O$ = $\frac{2\pi}{\lambda}$($\cos(\theta)\cos(\beta)$, $\cos(\theta)\sin(\beta)$, $\sin(\theta)$) = ($\frac{2\pi}{\lambda}$, 0, 0), respectively. The four $\beta$-scans were performed at the $\theta$-angles: (c) p1 (in black), (d) p2 (in black), (e) p4 (in blue) and (f) p3 (in blue), respectively. The top and bottom abscissas are $\beta$ (in deg.) and the parallel component, $q_{||}$ ($=\sqrt{q_x^2 + q_y^2}$) (in Å$^{-1}$), of the scattering vector, $\vec{q}$, respectively.
respectively. For example, for Β(x) at depth, x, \( \text{lat}_1 = c \) and \( \text{lat}_2 = c \). The symbol \( c_0 \) is the changing rate of lattice parameters in depth, which is determined by fitting the simulations to measured intensity distributions.

To determine the changing rate \( c_0 \) of the lattice parameters for the Si\(_{0.7}\)Ge\(_{0.3}\)/Si sample of a thousand atomic layers along [001], the multilayer dynamical theory of X-ray diffraction\(^\text{12}\) is employed to deal with multiple boundaries. The simulations start with Maxwell’s equations, whose solutions as Bloch functions leading to the Fundamental equations of wavefield, Supplementary equation (10) (See Supplement II) which can be solved as an eigenvalue equation by using the formalism in single Cartesian coordinates\(^\text{11}\). 4N modes with 4N eigenvectors and eigenvalues are involved in an N-beam diffraction with \( N \geq 2 \) (see Supplement III) for each atomic layer. By applying the boundary conditions, the continuities of the tangential components of the electric field, \( E_\theta \) and magnetic field, \( H_\phi \), and the normal components of the electric displacement, \( D_n \) and magnetic induction, \( B_n \) (Supplement IV), the diffracted E fields at the \( n \)th atomic layer are calculated as \( \phi = \sum_{j=1}^{4N} c_j N_{n,j} \), which is the sum of the 4N E-fields (eigenvectors) with the 4N proportional coefficients \( c_j \) and their corresponding phases, \( \phi_{n,j} \), at the top boundary (\( l = 1 \)) and bottom boundary (\( l = 2 \)) of the \( n \)th layer considered. For multilayers, the coefficients, \( c_j \) are solved by the boundary conditions for the top (entrance) surface, the intermediate boundary from \( n \)-th to \((n + 1)\)th layers, and the bottom (exit) surface of the sample. This leads to the diffracted E-fields given in Supplementary equation (33) (see, Supplement V). For each surface reflection the calculations involve 1000 atomic layers and 4N modes (\( N = 3 \) for three beam BSD) for each layer. Therefore a linear system of \( 4 \times 3 \times 1000 \) equations are simultaneously solved to give the calculated profiles (tth- and beta-scans) of the three surface reflections, 202, 022 and 422, respectively.

Moreover, due to the shallow diffraction angles of the surface reflections with respect to the crystal surface, part of the diffracted beams are absorbed by the crystal. Therefore a fitting function \( F_m^{(n)}(R(\text{tth, beta})) \) at the

![Figure 4. Measured and simulated intensity distributions.](image-url)
Figure 5. $\sigma$-Tensor elements vs. depth. (a) The three diagonal elements, $a_x$, $b_y$, and $c_z$, are plotted from the top (depth = 0 Å) to the thin-film, Si$_{0.7}$Ge$_{0.3}$ (until 597 Å), and the interface (597~750 Å), and finally the Si substrate. (b) The two elements $a_y$ and $a_z$ are the y- and z- components of the lattice unit vector, $a$. (c) The $b_x$ and $b_z$ are the x- and z-components of the lattice unit vector, $b$. (d) The $c_x$ and $c_y$ are the x- and y- components of the lattice unit vector, $c$. The corresponding strains, calculated according to the predicted lattice constants (See Supplementary Figure 4) from Vegard’s law and the EDS data, Fig. 1c, are: (e) the tensile strains, $\varepsilon_{xx}$, $\varepsilon_{yy}$ and $\varepsilon_{zz}$, (f) the shear strains, $\tau_{yx}$, $\tau_{zx}$, (g) $\tau_{xy}$, $\tau_{zy}$, (h) $\tau_{xz}$, $\tau_{yz}$. (See, Supplement IX). The error bars of the ordinates are estimated from the 1th partial derivative of Bragg’s law with respect to $\beta$ and $\theta$ (see, Supplement VIII). And the error bar of the abscissa is equal to the two times of the average roughness ($= \sigma_{\text{surface}} + \sigma_{\text{interface}} \approx 1$ nm), being about 20 Å. From the Si$_{0.7}$Ge$_{0.3}$ thickness measurements of the EDS (~57 nm, Fig. 2d), HRTEM (~59.9 nm, Fig. 2f), XRR (~58.5 nm, Fig. 2e) and BSD (~59.7 nm, here), the Si$_{0.7}$Ge$_{0.3}$ thickness could be concluded in the range about 57~60 nm.
position vector, \( \mathbf{R} \) (tth, beta), of the detector from the sample is given to each surface reflection, where the diffraction geometry, acceptance angle of the detector, beam divergence, and the miscut angle between the surface and atomic layers are considered (See, Supplement VI). The fitting functions are plotted in Supplement VII. The interference among the diffracted beams inside the crystal is also included. This leads to the diffracted intensity, \( I_m \), as below:

\[
I_m(\text{tth, beta}) = \left| \sum_{\Delta \alpha, \Delta \beta=1}^M \sum_{m=1}^{M} \sum_{n=1}^{M} E_{m}^{(n)} \left( \frac{1}{i \lambda} \mathcal{F}_{m}^{(n)}(\mathbf{K}_{m}(\mathbf{R}(\text{tth, beta}))-\mathbf{z}) \right) \right| \]

where \( E_{m}^{(n)} \) is the diffracted E-field of the \( n \)th layer's top boundary for the \( m \)th reflection. Note that \( m = 0 \) is for the forward diffracted beam O, \( m = 1 \) for the symmetric Bragg reflection G, and \( m = 2 \) for the surface diffraction L, and \( E_{m}^{(n)} \) and \( E_{m}^{(n)} \) are the vertical positions of the top and bottom boundaries of the \( n \)th layer. \( \mathbf{K}_{m}(\mathbf{R}(\text{tth, beta})) \) is the \( z \)-component of the wavevector \( \mathbf{K}_{m}(\mathbf{R}(\text{tth, beta})) \) outside the crystal of the \( n \)th layer's top boundary for the \( m \)th reflection. The terms, \( \Delta \theta (\sim -0.007 \text{ deg.}) \) and \( \Delta \phi (\sim -0.02 \text{ deg.}) \) are the vertical and horizontal divergences, respectively on the beamline BL17B1. The symbol, M is the total number of atomic layers of the simulation i.e, \( M = 1000 \). The position vector, \( \mathbf{R} \), is shown in Supplementary equation (35).

The best fit between the simulated intensity distributions to the measured ones is reached when \( \sigma_0 = 0.6 \) for these cases. When \( \sigma_0 < 0.6 \), the measured intensity distributions of the interference between the diffraction from the Si0.7Ge0.3 and from the Si substrate cannot be matched by the simulated curves. When \( \sigma_0 > 0.6 \), the simulated peak intensities at p1 and p4 will be off the measured values. With \( \sigma_0 = 0.6 \), the nine elements of the \( \sigma \) tensor as functions of depth in Å are determined, which are shown in Fig. 5a–d. The corresponding strains, Fig. 5e–h, are estimated with the expected ones which are predicted from the EDS data, Fig. 2d, and Vegard’s law (See, Figure 6. The six lattice parameters versus depth. (a) The three lattice parameters, a, b, and c vs depth. (b) The three lattice parameters, \( \alpha, \beta \) and \( \gamma \) vs depth. (c) The blow-up of Zone 1 in (a). (d) The blow-up of Zone 2 of (b). The error bars given in figure are estimated from the \( 1^{st} \) partial derivative of Bragg’s law with respect to tth and beta (see, Supplement VIII). In the region of the thin-film, Si0.7Ge0.3 (about 0–597 Å), the six lattice parameters, a, b, c, \( \alpha, \beta \) and \( \gamma \) are about 5.4269 \( \pm \) 0.00057 Å, 5.426 \( \pm \) 0.0023 Å, 5.534 \( \pm \) 0.0024 Å, 90.07 \( \pm \) 0.04°, 89.85 \( \pm \) 0.012° and 90.0193 \( \pm \) 0.0060°, respectively. The lattice parameters at the interface (around 664 Å in depth) are roughly 5.4273 \( \pm \) 0.0006 Å, 5.425 \( \pm \) 0.0023 Å, 5.4820 \( \pm \) 0.0024 Å, 90.080 \( \pm \) 0.024°, 89.879 \( \pm \) 0.012° and 90.018 \( \pm \) 0.006°. That of the silicon substrate (the depths are roughly larger than 745 Å) are approximately 5.42796 \( \pm \) 0.00057 Å, 5.425 \( \pm \) 0.0023 Å, 5.430 \( \pm \) 0.0023 Å, 90.092 \( \pm \) 0.024°, 89.912 \( \pm \) 0.012° and 90.016 \( \pm \) 0.0060°. The c-axis of the thin-film, Si0.7Ge0.3, is gradually decreased in the interface and reaches the Si value below the interface. While the lattice parameters, a, b, and c of the Si0.7Ge0.3 and silicon substrate are nearly the same for all depths.
Supplement IX). The uniqueness of lattice parameter determination is also verified (See, Supplement X), such that the determined lattice parameters fit all the BSD measurements simultaneously.

Furthermore, the six lattice parameters can be also calculated from the $\sigma$-tensor. The results are shown in Fig. 6a-b, and the blow-ups of the interface in Fig. 6c-d. After the thin film deposition, the parameter $\alpha$ is slightly larger and $\beta$ is slightly smaller than 90 degrees indicating that the c-axis deviates from the normal direction, [001], due to the thin-film growth so that the two angle, $\alpha$ and $\beta$ are not exactly equal to 90° ($\sigma$ ≥ 90° and $\beta$ ≤ 90° in all depths). Due to the growth direction perpendicular to the [100] or [010], the variation of the angle, $\gamma$, is the smallest. When the thin-film, Si$_{0.7}$Ge$_{0.3}$, are grown on the silicon wafer, the a- and b-axis of the thin-film, Si$_{0.7}$Ge$_{0.3}$, are bound to the silicon substrate. To relax the strain, the c-axis of the thin-film, Si$_{0.7}$Ge$_{0.3}$, is longer than a- and b-axis, and the structure became rectangular rather than cubic$^{16}$. Also, the silicon substrate inside the probing limit (~300 nm) is slightly distorted as a triclinic structure, and its c-axis is stray from the direction, [001] due to the thin-film deposition.

In conclusion, the depth profiles of interfacial strains and lattice parameters of Si$_{0.7}$Ge$_{0.3}$/Si are successfully obtained. This method can be used for strain mapping of a wide variety of multilayer crystal systems (For imperfect multilayers, the simulations can be replaced by the power-transfer equation of the kinematical theory$^{17}$), which is useful for polarization engineering in ferroelectricity$^{18}$ and nanotechnology applications$^{19–25}$. Especially, the shear and tensile strains may be applied to offer sufficient information to control the interfacial carrier mobility in the so-called stain-engineering$^{26–30}$ for devices. With the advent of new X-ray sources beyond diffraction-limit, the BSD of better coherence may improve the strain resolution further.

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Acknowledgements
We are indebted to the Ministry of Science and Technology (MOST) and Ministry of Education (MOE) for the financial supports, including the Academic Summit programs. We thank also the National Tsing Hua University, National Synchrotron Radiation Research Center and National Nano Device Laboratory for laboratory assistances, beam time arrangements, and sample preparation, respectively. Special thanks are given to National Center for High-Performance Computing (NCHC) for providing computer clusters for all the simulation work.
The assistance and help from M.-T. Tang, H.-T. Jeng, T.-S. Wu, J.-H. Yen, Y.-W. Tsai, S.-C. Weng, Y.-Y. Chang, W.-C. Liu, Y.-H. Wu, P.-Y. Liao, Y.-T. Ye, Y.-C. Chen, and H. Liang are also gratefully acknowledged.

Author Contributions
Y.-Z.Z. designed and performed the experiments, and prepared the numerical calculations to analyze the experimental data, and wrote the paper. S.-L.C. proposed the research direction, participated in experimental discussion and data analysis, and wrote the paper. Y.-L.S. participated in discussion and provided critical comments.

Additional Information
Supplementary information accompanies this paper at http://www.nature.com/srep

Competing financial interests: The authors declare no competing financial interests.

How to cite this article: Zheng, Y.-Z. et al. Depth profiles of the interfacial strains of Si$_{0.7}$Ge$_{0.3}$/Si using three-beam Bragg-surface diffraction. Sci. Rep. 6, 25580; doi: 10.1038/srep25580 (2016).

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