Characterization of strain fields in Si1-xGex island structures by means of quantitative high-resolution electron microscopy

Anh Tuan Tham, Reinhard Otto, Wolfgang Neumann, Herbert Wawra, HP Strunk

Microsc. Microanal. 9 (Suppl. 3), 2003
DOI: 10.1017/S1431927603023328

Characterization of strain fields in $Si_{1-x}Ge_x$ island structures by means of quantitative high-resolution electron microscopy

Anh Tuan Tham[1], Reinhard Otto[1], Wolfgang Neumann[1], Herbert Wawra[2] and H.P. Strunk[3]

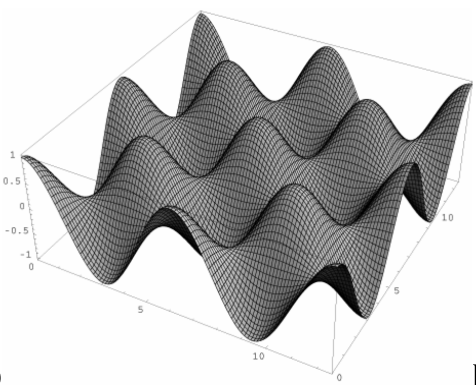
[1]Humboldt University of Berlin, Institute of Physics, Chair of Crystallography,
Newtonstr. 15, 12489 Berlin, Germany
[2]Institute of Crystal Growth, Max-Born-Str. 2, 12489 Berlin, Germany
[3]Friedrich-Alexander-University Nürnberg - Erlangen, Institute of Microcharacterisation,
Cauerstraße 6, 91058 Erlangen, Germany

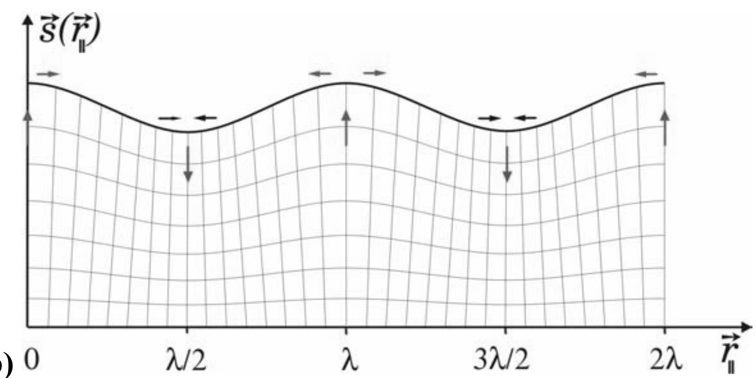
$Si_{1-x}Ge_x$ layers were grown heteroepitaxially on (001)-oriented Si substrates by liquid phase epitaxy close to the thermodynamic equilibrium, i.e. with very low growth driving force, in the Stranski-Krastanow mode. The large strains often associated with lattice mismatching provide a significant reservoir of elastic energy that can be released to drive structural and morphological evolution of the growing film. Strain relaxation via surface roughening [1,2] and afterwards nucleation of three-dimensional faceted islands can precede the conventional mode of strain relaxation via dislocation formation. Starting from the theoretical consideration of surface rippling in a thin layer under biaxial strain [3] a model for the growth mechanism of the island structure based on the state of strain fields in substrate areas surrounding and beneath the islands could be developed [4]. This was established by strain mapping analyses with the DALI program [5] on HRTEM images of such areas.

Surface ripples in (Si,Ge)/Si systems occur in <100> soft directions that have small elastic constants and form a sinusoidal ripple pattern (fig. a). The wavelength λ of such a modulation scales with $\lambda \sim \sigma^{-2} \sim \varepsilon^{-2} \sim f^{-2} \sim x^{-2}$ (σ: strain, ε: deformation, f: misfit and x: Ge-amount). λ is constant during further material deposition whereas its amplitude is continuously increasing. The strain is reduced at the peaks of the structure while it is increased in the troughs. Simultaneously, the total surface energy is increased because of the modulation. Surface rippling is accompanied by local bending of lattice planes in both layer and substrate (fig. b), respectively. In further growth stages pseudomorphous islands nucleate on the relaxed peaks of the ripple pattern. The islands arrange therefore favourable in <100> directions and exhibit a truncated pyramidal shape with {111} side facets. The nucleation of such islands requires firstly the same local layer thickness, and secondly the same local gradient of lateral distortion components at the positions corresponding to island's edges and corners. From the consideration of the quadratic base of the islands theoretical calculations supply the lateral size w of such islands which is uniformly about 0,41λ. The phenomena of self-limiting and self-assembling in (Si,Ge)/Si island structure could be proved. Moreover the ratio between gradients of vertical distortion components at the corner and edge of an island could be calculated and is amounting to the geometrical factor $\sqrt{2}$ [6].

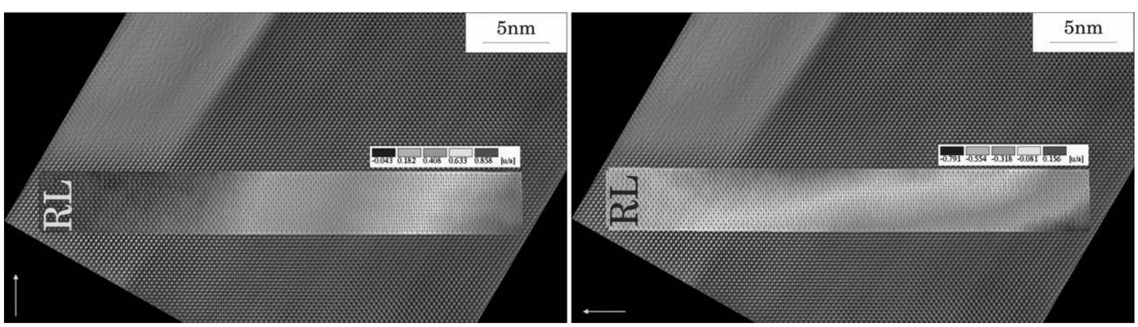
Analyses of strain states in substrate areas beneath island edges (fig. c) and corners (fig. d) illustrate and support all those model calculations. The waving form of lateral (001) lattice planes and the bending of vertical {220} and {400} ones could be clearly shown. The experimentally determined ratio between gradients of vertical distortion components at the island corner and edge of about 1,39 is consistent with the theoretical considerations. In additional systematic measurements of lateral island sizes and distances between them, in samples with high Ge-amount and high ordering of islands, yield $w \approx 0{,}44\lambda$. The growth mechanism of such a (Si,Ge)/Si island structure could be cleared up and verified [6].

References:
[1] R. J. Asaro and W. A. Tiller, Metall. Trans. A **3**, 1789 (1972).
[2] M. A. Grinfeld, Sov. Phys. Dokl. **31**, 831 (1987).
[3] D. J. Srolovitz, Acta Metall. **37**, 621 (1989).
[4] A. T. Tham, R. Otto, I. Häusler, A.-K.Gerlitzke, H. Wawra, M. Lentzen, H. Kirmse, W. Neumann, H. P. Strunk and K. Urban, Suppl. Z. Krist. **20**, 38 (2003).
[5] A. Rosenauer, S. Kaiser, T. Reisinger, J. Zweck, W. Gebhard and D. Gerthsen, Optik 102, 63 (1996).
[6] A. T. Tham, R. Otto, W. Neumann, H. Wawra and H. P. Strunk, in preparation.

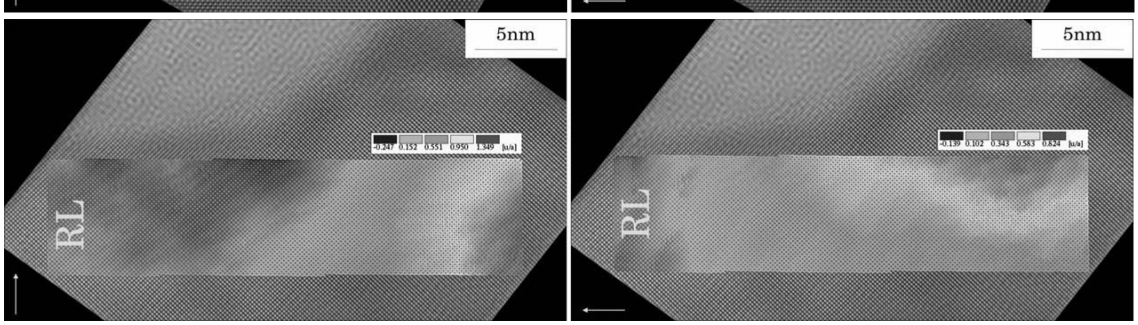

a)



b)



c)



d)

Figures: (**a**) Illustration of sinusoidal ripple pattern and of (**b**) modulated surface and accompanying distorted lattice planes; (**c**) + (**d**) DALI strain analyses in substrate areas beneath island edge and corner with reference lattices (RL) on the left side show the alterations of vertical (l.) and lateral (r.) distortion components in cross-sectional samples. From left to right the vertical distortion increases, whereas the lateral one reaches maximum values immediately beneath the border of island base.