# 論文の内容の要旨

論文題目

# Epitaxial Growth of Ge Layer with Low Threading Dislocation Density on Si Substrate for Light-Emitting Device Applications

（発光素子応用に向けたSi基板上低貫通転位密度Ge層のエピタキシャル成長）

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The objective of this work is to establish a novel method to reduce dislocations in germanium (Ge) epitaxial layers on silicon (Si) for light source applications. This dissertation describes a proposal of novel dislocation reduction model, numerical calculations of dislocation reduction, experimental verifications for reduction of dislocations, direct observations of dislocations by transmission electron microscopy (TEM), and a feasibility study for light source applications.

Silicon photonics has been considered to be a promising technology to enable high-speed, large-capacity, and low-cost communication networks. For the practical application of silicon photonics technology, the development of on-chip light sources has been one of the most challenging issues fundamentally because of the indirect band structure of Si.

As a candidate for an on-chip light source material, a tensile-strained n-type Ge was theoretically proposed in 2007, and first Ge laser diode (LD) was reported in 2012. Ge can emit (and detect) light around 1.55 µm, corresponding to the optical communication wavelength, and is compatible with Si complementary metal oxide semiconductor processing. However, reported Ge LDs have shown large threshold current densities ($J_{th}$); almost two orders of magnitude higher than the theoretical prediction.

The major cause of the large $J_{th}$ lies in defect-assisted non-radiative recombination (NRR) in Ge layers and at Ge surfaces. Although NRR at Ge surfaces is suppressed by thermal oxidation,

it is required to reduce defects in Ge for light source applications. In the case for Ge epitaxial layers on Si, threading dislocations (TDs) are formed owing to lattice-mismatch between Ge and Si as large as 4.2 %, and the density of TDs is as high as 10 to the $9^{th}$ power. Although many methods have been tried to reduce TDs in Ge epitaxial layers on Si, the previous methods have drawbacks to light source applications in terms of dopant out-diffusion and/or optical confinement in Ge. Thus, a novel TDD reduction method is required for light source applications, i.e., to reduce $J_{th}$ in Ge LDs.

In this dissertation, a novel method for dislocation reduction is proposed employing image force and selective epitaxial growth (SEG) technique. A theoretical model is proposed, and numerical calculations are performed based on the theoretical model. The TD reduction occurs as following steps:

(1) TDs are bent to be normal to growth surfaces owing to image force, which is an attractive force between dislocations and free surfaces,

(2) bent TDs turn toward bottom Ge/Si interfaces as Ge SEG proceeds, and

(3) some TDs are terminated at the bottom Ge/Si interfaces where SEG Ge layers coalesce each other, resulting in reduction of TDs penetrating to the top Ge surface.

The numerical calculations show that the rate of TDs terminated at the bottom Ge/Si interfaces is determined by aperture ratio of SEG mask, i.e., the ratio of Ge growth area. According to the calculation, TD density is reduced by a factor of 1/100 where aperture ratio is as small as 0.1.

Experimental verification of the theoretical model is carried out in 3 steps.

First, Ge growth in lateral direction over $SiO_2$ masks is investigated by cross-sectional scanning electron microscopy (SEM) observations. It is found the growth rate of Ge in lateral direction depends on the width of Ge growth area, which indicate that the Ge growth in lateral direction is dominated by the Ge facets of the slowest growth rate; {113} facets. As a result, it is found that SEG Ge layers coalesce when both the width of Ge growth area and the width of $SiO_2$ masks are narrow enough, finally forming flat-top films (coalesced Ge).

Then, experimental verification of TD reduction is performed employing etch pit density measurement method. It is revealed that the TDs in coalesced Ge is reduced as theoretically predicted. In addition to the reduction of TDs, distribution of the TDs penetrating to the top surface well reproduces the theoretical model. TD density as low as 4 times 10 to the $7^{th}$ power is obtained in coalesced Ge, where aperture ratio is 0.6. This TD density is two orders of magnitude lower than that in ordinary Ge epitaxial layers on Si.

Finally, TEM observations are performed to observe TDs in coalesced Ge. Cross-sectional

TEM observations reveal that the reduction of TDs actually occurs in coalesced Ge as predicted by the theoretical model. Plan-view TEM observations directly show that TD density in coalesced Ge is lower than that in blanket Ge. In addition to the behavior of TDs predicted by the theoretical model, cross-sectional TEM observations reveal that generation of TDs in coalesced Ge, and plan-view TEM observations reveal that there are TDs inclined to be parallel to $SiO_2$ masks in coalesced Ge. Both unpredicted behaviors of TDs are, however, understandable considering image force and slight misorientation among SEG Ge layers.

At the last part of this dissertation, a feasibility study for light source applications are carried out through photoluminescence (PL) measurements and optical pumping measurements.

Prior to the measurements, tensile strain and n-type doping in coalesced Ge are investigated. Tensile strain is induced in coalesced Ge owing to the mismatch of the thermal expansion coefficients between Ge and Si. N-type doping in coalesced Ge is performed by a thermal diffusion of phosphorus (P). Both tensile strain and n-type doping level are enough for light source applications. In addition to that, simulation of optical propagation mode in coalesced Ge reveals that coalesced Ge has advantage over conventional structure in terms of less light intensity at defective Ge/Si interfaces.

PL measurements are carried out before and after the P thermal diffusion. PL measurements before the diffusion suggests that there are NRR centers in coalesced Ge, which is not TDs, and the NRR centers is removed during the P diffusion process.

Fabry-perot (FP) resonators are fabricated using the coalesced Ge layers, and optical pumping measurements are carried out on the FP resonators. Clear threshold behaviors are observed with the threshold power densities around 18 kW/cm$^2$. The observed thresholds are smaller than reported threshold in an optically pumped Ge laser, although it is still difficult to conclude that the threshold behaviors are laser operation because amplified spontaneous emission also shows threshold behavior.

In summary, a novel method to reduce dislocations in Ge epitaxial layers on Si is theoretically proposed and experimentally verified. A feasibility study for light source applications show promising results, i.e., threshold power densities lower than conventional Ge epitaxial layer on Si are observed. Further reduction of dislocations and laser operation is expected based on the method proposed and verified in this dissertation.