# Direct laser writing of graded-index SiGe waveguides via phase segregation

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## ABSTRACT

We report direct laser writing of graded-index optical waveguides via phase segregation in initially homogenous silicon-germanium (SiGe) thin films epitaxially-grown on silicon substrates. We used a continuous wave (CW) laser operating at a wavelength of 532 nm. The laser beam was focused to a 5 µm diameter spot on the surface of SiGe films with a thickness of 575 nm and a Ge concentration of %50. Compositional separation of a SiGe film was induced by melting the surface, and the composition profile was tailored by controlling the scan speed of the laser-induced molten zone in a range of 0.1-200 mm/s. At high scan speeds, scanning the laser beam produces a travelling Ge-rich molten zone, where a build-up of Ge content occurs at the trailing edge because of insufficient diffusion-limited Ge transport. Material characterizations have revealed that the laser-processed SiGe microstripes consist of Ge-rich strip cores (> 70% Ge) surrounded by Si-rich under-claddings (<30% Ge). Scan-speed dependent phase segregation allows for fabrication of graded-index SiGe waveguides with tunable compositional profiles, which were characterized by optical transmission measurements, and modal analysis using simulations. Our method could also be applied to pseudo-binary alloys of ternary semiconductors (AlGaAs), which have equilibrium phase diagrams similar to that of SiGe alloys.

**Keywords:** Binary semiconductor alloys, epitaxially-grown thin films, silicon-germanium, phase segregation, direct laser writing, graded-index waveguide, phase-field modeling, laser materials processing.

## 1. INTRODUCTION

Incorporation of germanium into silicon has a great prospect not only for microelectronics, but also for photonics.[1] The biggest advantage of alloying is that the optical and electrical properties of a $Si_{1-x}Ge_x$ alloy such as refractive index, mobility, and electronic bandgap can be tuned through the composition by changing the Ge fraction $x$.[2] Furthermore, Si/SiGe and Ge/SiGe heterostructures have recently been drawing increasing interest for the fabrication of modulators, detectors, and light sources.[3,4] Therefore, SiGe alloys have been extensively used in various fields for different applications, for example heterojunction bipolar transistors in electronics; photodetectors, solar cells, and thermoelectric generators in thermo-photovoltaics.[5] Last, but not least, SiGe alloys are also promising materials for quantum cascade lasers, mid-infrared (mid-IR) optical waveguides, optical interconnects, and many other applications in photonics and nonlinear optics.[6] As SiGe is a complementary metal-oxide-semiconductor (CMOS) compatible material, it can also be used as an integration platform for the convergence of electronics and photonics, where various components can be produced on-chip.

Conventional waveguides for integrated platforms depend on patterning of silicon-on-insulator (SOI) wafers by e-beam lithography and etching. This approach provides compact components for use in the telecom range, however, the silica buffer oxide layer in SOI platforms suffers from strong absorption above 3.6 µm, hindering photonic applications in the mid-IR range. Therefore, graded-index SiGe waveguides have recently received increased interest for mid-IR applications in integrated photonics, due to the low optical losses (1-2 dB/cm) in the wavelength range of 2-8 µm. To date, two approaches have been demonstrated for the fabrication of SiGe waveguides on silicon platforms. 1) Incorporation of germanium into silicon substrates by using either diffusion or ion implantation.[7,8] Despite the low loss (<0.5 dB/cm) waveguides obtained by diffusion, this method has not been widely adopted as the thermal processing requires very long durations (> 60h at 1200 °C), in addition to the deposition and lithographical patterning of a Ge-rich strip source on silicon, as schematically shown in Fig. 1a. 2) Graded SiGe waveguides can also be directly fabricated by epitaxial growth and lithographical patterning,[9,10] as schematically shown in Fig. 1b. However, these have two drawbacks: i) The graded refractive index can only be obtained in the growth direction, which is perpendicular to the substrate surface, and a step index profile in the plane still requires patterning of the surface for mode confinement similar to the conventional SOI waveguides. ii) Waveguides with different graded index profiles on the same substrate require different growth processes for each of them, increasing the cost and complexity of the integration process.

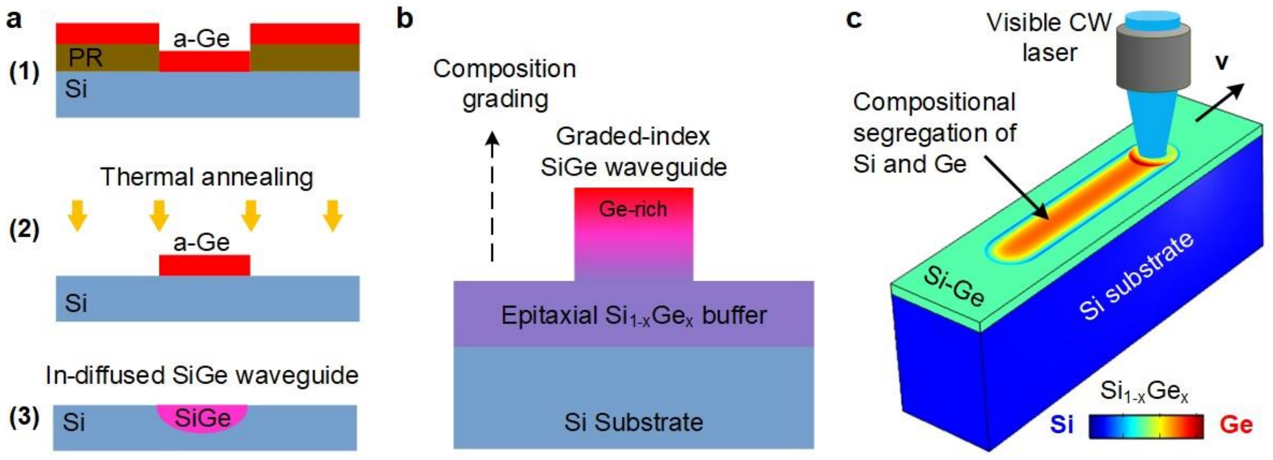


Figure 1. Methods for fabrication of graded-index SiGe waveguides. a) Deposition of Ge through a mask and subsequent thermal annealing to in-diffuse Ge into a silicon substrate. b) Epitaxial growth of graded-composition SiGe film on a SiGe buffer layer, and subsequent lithographical patterning and etching. c) Another approach proposed for the waveguide fabrication in this work, which is based on laser-driven phase segregation of an initially homogenous epitaxially-grown SiGe thin film resulting in a Ge-rich strip core and a Si-rich under-cladding. The compositional profile, and thus the index-profile of the SiGe waveguides are tuned by controlling the scan speed.

Capitalizing on our recent work,[11] we propose another approach to fabricate graded-index waveguides with Ge-rich strip cores, exploiting laser-driven phase segregation in homogenous Si-Ge thin films, as schematically shown in Fig. 1c. In the laser-written graded-index SiGe waveguides, an index grading both in the transverse and vertical directions is simultaneously achieved via compositional segregation of the SiGe within the laser-melt region. Moreover, this graded index profile is tunable by controlling the laser scan speed, allowing fabrication of customized waveguides using the same initially homogenous SiGe epilayer. An index profile customizable for each waveguide can be leveraged for dispersion engineering in nonlinear optical applications, instead of changing the size and shape of the waveguides. Furthermore, laser-driven compositional segregation in SiGe epilayers could enable a refractive index difference $\Delta n$ on the order of $10^{-1}$, which is higher compared to those obtained in laser-written waveguides in bulk silicon ($10^{-4}$) using pulsed-laser-induced modifications.[12] Direct laser writing of SiGe waveguides does not require lithographical patterning, eliminating scattering losses due to the roughness of the etched waveguide boundaries.

## 2. LASER PROCESSING OF SIGE EPILAYERS

### 2.1 Experimental setup

Our laser processing setup is schematically shown in Fig. 2. The thermal source is a laser (IPG-GLR-10W) CW radiation at a wavelength of 532 nm with a maximum power of 10 W. To avoid distortion in the laser beam, the optical power was adjusted by using a polarization beam splitter and a half-wave plate (HWP). The laser beam was focused on the top surface of the SiGe epilayer using a 10× objective lens (NA-0.25) to produce a spot size of 5 µm in diameter. A dichroic mirror was used to couple a collimated white light source into the optical path. By adjusting the position of the tube lens in front of the CCD camera, the laser and illumination sources were focused to the same point, allowing for in situ monitoring of the surface by using the CCD camera during the laser processing. Samples were mounted with a vacuum holder on high-precision motorized stages (Aerotech, ABL-1500), which are capable of movements in three dimensions (3D). These stages were used to scan the sample under the laser beam at speeds ranging from 0.1 to 200 mm/s. The power was adjusted between 1-3 W. High temperatures up to 1600 °C, sufficient to melt the semiconductor alloy epilayer, can be reached due to the high optical absorption of SiGe alloy in the visible spectrum.

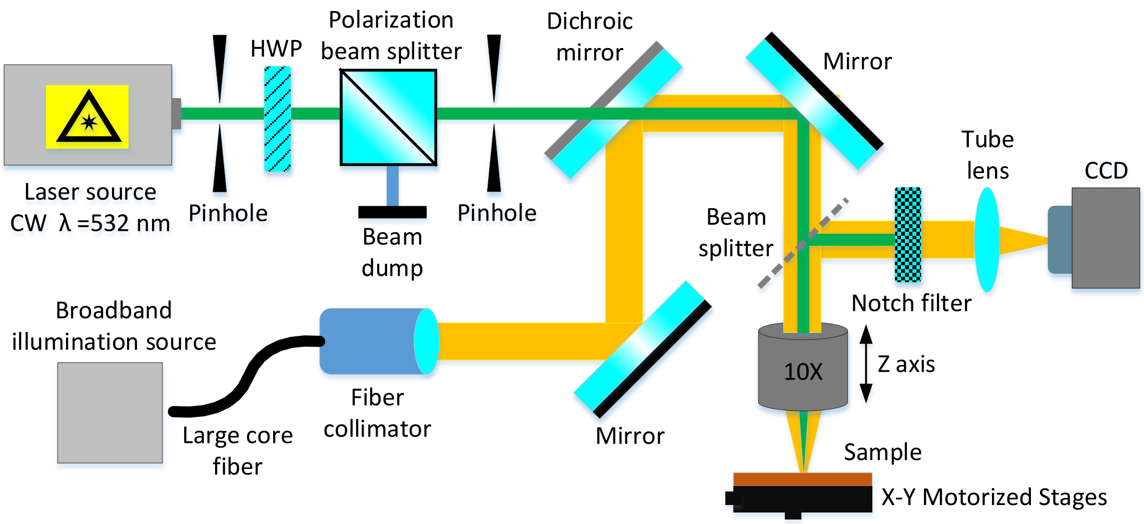


Figure 2. Schematic of the experimental setup used for laser writing of graded-index waveguides in SiGe thin films epitaxially grown on Si substrates. HPW, half-wave plate.

### 2.2 Laser writing of graded-index waveguides at various constant scan speeds

We begin our experimental work by applying laser processing on homogenous SiGe epilayers with a thickness of 575 nm and a Ge concentration of 50%. The $Si_{0.5}Ge_{0.5}$ epilayers were epitaxially-grown on silicon substrates by reduced pressure chemical vapor deposition (RPCVD). The laser beam with a power of 2.5 W was focused to a spot with a diameter of 5 µm on the surface of the $Si_{0.5}Ge_{0.5}$ epilayer by a 10× microscope objective. Laser processing was conducted at the same power, but with different constant scan speeds in the range of 0.1-200 mm/s. Scanning the stage under the fixed laser beam produces a travelling laser-induced molten zone, where phase segregation of SiGe occurs at the liquid/solid interface. Depending on the scan speed, the laser-driven phase segregation produces SiGe microstripes solidified with varying Ge compositions on the top surface, as shown in the optical microscope image in Fig. 3a. The laser-written SiGe microstripes for the low scan speeds of 0.1 and 1 mm/s are barely visible; however, wider microstripes emerge with a yellow/orange color as the scan speed increases. Ge accumulates on the surface at high scan speeds.

## 3. SIMULATIONS

We carried out 3D finite-element-method (FEM) based non-isothermal phase-field simulations incorporating laser-induced thermocapillary convection.[13] The Navier-Stokes equations were solved concurrently with the heat transport and segregation-diffusion equations. To reduce the computational cost, we chose a beam spot size of 2 µm and a scan range of 10 µm, which are smaller in size compared to the actual experimental parameters (5.7 µm and 4 cm, respectively). The other parameters used in the simulations were: optical power of 200 mW, scan speeds in the range of 1-500 mm/s, and a $Si_{0.5}Ge_{0.5}$ epilayer with a thickness of 500 nm (the experimental value is 575 nm). We also assumed that the thermal properties of the $Si_{1-x}Ge_x$ alloy such as the melting temperature and thermal conductivity are determined by the initial composition $x_0$=0.5. The values used for the material and thermal properties of the SiGe alloys were taken from the literature. The simulation results presented in Fig. 3b show the spatial redistribution of the Ge content (molar fraction $x$) within the laser-written SiGe microstripes at various constant scan speeds after laser processing. The laser-induced molten zone (red) travels along the scan direction dragging the Ge-rich liquid, and solidifies at the trailing edge with a scan-speed-dependent redistribution of the composition. After a short Si-rich transient (blue), an indefinitely long steady-state region emerges with a Ge-rich ($x > 0.5$) strip core (yellow/orange) and a Si-rich ($x < 0.5$) under-cladding. The phase-field modelling provides good qualitative agreement when compared to the experimental observations.

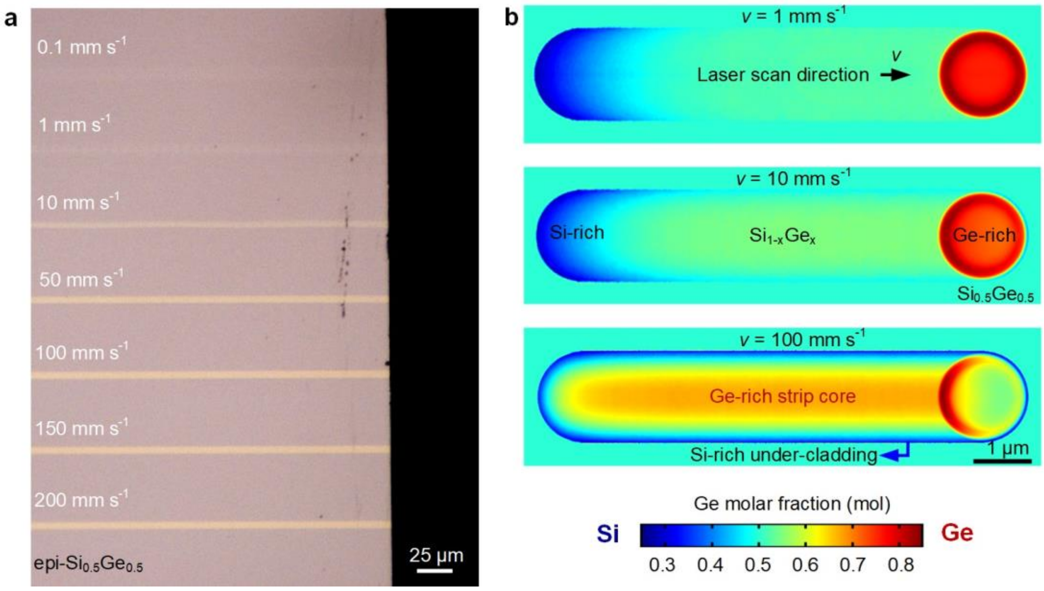


Figure 3. Laser writing of graded-index SiGe waveguides via scan-speed-dependent redistribution of initial composition. a) Optical microscope image showing a series laser-written microstripes on a $Si_{0.5}Ge_{0.5}$ epilayers, for scan speeds in the range of 0.1-200 mm/s. b) Results of FEM-based phase-field simulations for laser-driven phase segregation are given as composition color maps showing the Ge molar fraction *x* for the short transient (blue) and steady-state regions (yellow-orange) solidified behind the laser-induced molten zone (red) travelling at a constant scan speed in the range of 1-500 mm/s.

## 4. MATERIAL CHARACTERIZATION

To conduct a quantitative comparison, the cross-section of a SiGe microstripe written at a scan speed of 200 mm/s, was analyzed using scanning tunneling electron microscopy (STEM) with energy dispersive X-ray spectroscopy (EDX). A high-angle annular dark-field (HAADF) image shows the material contrast in Fig. 4a. The redistribution of the composition in the re-solidified region is given by the 2D EDX map in Fig. 4b. Our simulated result was calculated neglecting thermocapillary convection, but using the actual experimental sizes. Fig. 4c shows the simulated $Si_{1-x}Ge_x$ composition at the cross-section showing the 2D spatial redistribution of Ge in the Ge-rich core and Si-rich cladding.

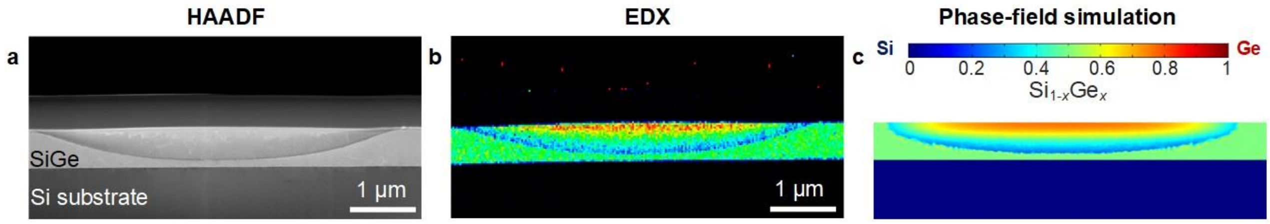


Figure 4. Elemental analysis of a SiGe waveguide laser-written at a scan speed of 200 mm/s. a) High-angle annular dark-field image (HAADF) showing the material contrast at the cross-section of the laser-melted region. b) EDX and c) FEM-based phase-field simulation results showing spatial redistribution of the composition at the cross-section for the sake of comparison. The color bar applies to both figures in (b,c).

## 5. MODAL ANALYSIS AND OPTICAL CHARACTERIZATION

We solved Maxwell's equations in the frequency domain to calculate the optical modes supported by a graded-index SiGe waveguide written at a scan speed of 200 mm/s by a focused beam of 2 µm in diameter. The 2D Ge molar fraction at the cross-section of the laser-written SiGe microstripe was obtained by a phase-field simulation, as given in Fig. 5a. As the process temperatures (1600 °C) are high enough to melt the surface, residual biaxial tensile strains occur within the laser-processed SiGe thin films, due to the difference between the thermal expansion mismatch between Ge and Si. The residual tensile strains can be as high as 0.6%, as demonstrated recently.[11] Therefore, photo-elastic effects, which are strain-induced changes in the refractive index need to be incorporated.[14] We found that an increase of 3% in the refractive index within the laser-melted strained region gives the best agreement with the optical transmission measurements in terms of matching the mode profiles. The resulting refractive index profile $n(x)$, which depends on the Ge content $x$,[15] and photo-elastic effects, is shown in Fig. 5b. The simulated fundamental mode profile for the transverse electric (TE) polarized mode of light at a wavelength of 2 µm is shown in Fig. 5c.

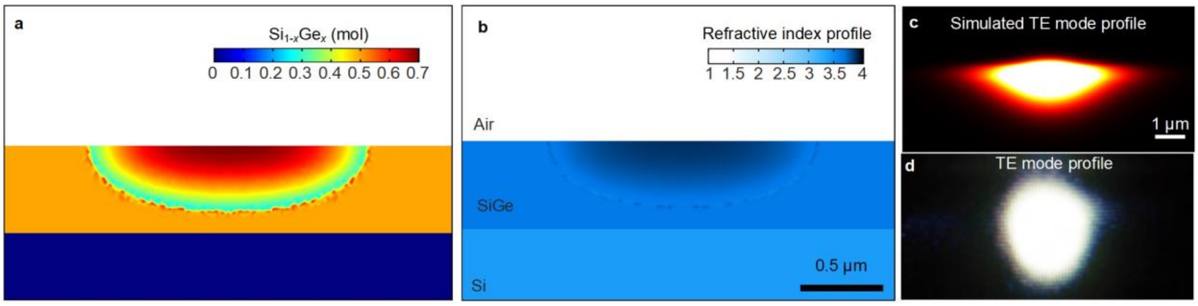


Figure 5. Modal analysis and optical characterization of laser-written graded-index waveguides. a) Simulated spatial redistribution of Ge molar fraction $x$ and b) calculated refractive index of a SiGe waveguide laser-written at a scan speed of 200 mm/s. Simulated c) TE and mode profile obtained by modal analysis using the refractive index profile in (b). IR camera image showing the intensity profiles for the d) TE mode, which was captured by an IR camera.

For a proof-of-principle experimental demonstration, we used a 1 cm long SiGe microstripe that was written using a laser with a spot size of 5 µm at a scan speed of 200 mm/s. The end facets were prepared for optical coupling by manual cleaving, and a fiber laser emitting light at a wavelength of 2 µm was free space coupled to the waveguide by using a 60× objective. The light at the output was then collimated by a 40× objective and imaged by infra-red (IR) camera, which captured an image of the TE polarized mode shown in Fig. 5d. Similar experiments were also conducted for the fundamental TM mode, which also showed good agreement with the simulations, and we observed (both simulations and experiments) that only the fundamental modes were coupled and guided through these laser-written SiGe waveguides at a wavelength of 2 µm. Moreover, optical guiding was observed even for the waveguide written at the lowest scan speed of 0.1 mm/s, where the least compositional separation within the laser-written SiGe microstripe was obtained. This observation reveals that the residual tensile strains increase the refractive index in the laser-processed regions.

## 6. CONCLUSIONS

In conclusion, we have demonstrated direct laser writing of graded-index waveguides within SiGe epilayers by controlling phase segregation during directional solidification through the laser scan speed. 3D FEM-based non-isothermal phase-field simulations including the effects of thermocapillary convection were carried out to investigate the laser processing of SiGe epilayers. We also provided experimental support for laser-driven phase segregation in $Si_{0.5}Ge_{0.5}$ films epitaxially grown on silicon substrates, and demonstrated optical coupling into laser-written graded-index SiGe waveguides at a wavelength of 2 µm. As a future work,[13] we will investigate formation of in-plane transverse SiGe superlattices within waveguides by modulation of the laser power and beam position during laser processing at constant stage scan speeds. On-chip, post-process laser writing of waveguides and periodic compositional grating structures within semiconductor alloy epilayers could pave the way for new device designs and applications in the fields of optoelectronics and photonics.

## ACKNOWLEDGEMENT

The authors acknowledge the use of the IRIDIS High-Performance Computing Facility at the University of Southampton, and support of the Engineering and Physical Sciences Research Council (EPSRC) (EP/P000940/1 and EP/N013247/1) for the completion of this work.

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