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Research Article

Thermophysics Simulation of Laser Recrystallization of High-Ge-Content SiGe on Si Substrate

Chao Zhang,[1] **Jianjun Song**,[2] **Jie Zhang**,[2] **and Shulin Liu**[1]

[1]*School of Electrical and Control Engineering, Xi'an University of Science and Technology, Xi'an 710054, China*
[2]*Key Lab of Wide Band-Gap Semiconductor Materials and Devices, School of Microelectronics, Xidian University, Xi'an 710071, China*

Correspondence should be addressed to Chao Zhang; zhangchao@xust.edu.cn

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The high-Ge-content SiGe material on the Si substrate can be applied not only to electronic devices but also to optical devices and is one of the focuses of research and development in the field. However, due to the 4.2% lattice mismatch between Si and Ge, the epitaxial growth of the high-Ge-content SiGe epitaxial layer directly on the Si substrate has a high defect density, which will seriously affect the subsequent device performance. Laser recrystallization technique is a fast and low-cost method to effectively reduce threading dislocation density (TDD) in epitaxial high-Ge-content SiGe films on Si. In this paper, by means of finite element numerical simulation, a 808 nm laser recrystallization thermal physics model of a high-Ge-content SiGe film (for example, $Si_{0.2}Ge_{0.8}$) on a Si substrate was established (temperature distribution physical model of $Si_{0.2}Ge_{0.8}$ epitaxial layer under different laser power, $Si_{0.2}Ge_{0.8}$ epitaxial layer thickness, and initial temperature). The results of this paper can provide important technical support for the preparation of high-quality high-Ge-content SiGe epilayers on Si substrates by laser recrystallization.

1. Introduction

In order to improve the performance of MOS devices and continue Moore's Law, various new materials and new technologies are emerging. High-Ge-content SiGe on Si substrate has high carrier mobility, is compatible with Si process, and has better interface characteristics than Ge material on Si substrate and has become one of the semiconductor materials for high speed/high performance MOS device research and application [1, 2]. In addition, the high-Ge-content SiGe material has an absorption wavelength of up to 1.55 μm in the near-infrared region, which is suitable for the development of optical devices such as infrared detectors [3, 4]. The development of high-Ge-content SiGe on Si substrates has become one of the focuses of research and development in the field.

High-quality, high-Ge-content SiGe alloys on Si substrates are the "material basis" for applications; however, due to a 4.2% lattice mismatch between Si and Ge, it is very difficult to directly heteroepitaxially grow a high-quality SiGe alloy on a Si substrate [5]. The higher the Ge composition of the SiGe alloy epitaxial layer, the greater the mismatch rate with the substrate Si. The lattice mismatch on the one hand causes island-like growth, which increases the surface roughness of the high Ge composition SiGe epitaxial layer [6]. On the other hand, it causes high threading dislocation density (TDD) in the SiGe layer. In the high-Ge-content SiGe epitaxial layer, either a closed dislocation loop is formed or a pair of screw dislocations extend longitudinally to the outer surface of the high-Ge-content SiGe epitaxial layer, which decreases the crystal quality of the epitaxial layer and degrades the device performance [7]. Therefore, how to solve the problem of preparing high-quality and high-content SiGe epitaxial layer on Si substrate deserves attention and further research.

From the above, it is difficult to obtain high-quality, high-content SiGe epitaxial layer due to the large lattice mismatch between Si and Ge. Interfacial dislocation defects continuously extend longitudinally to the surface of the epitaxial layer during the gradual thickening of the epitaxial layer, thereby resulting in a decrease in the lattice quality of the epitaxial layer. Laser recrystallization technique (shown in Figure 1) provides an effective method to solve this problem [8]. The high-Ge-content SiGe epitaxial layer directly prepared on the

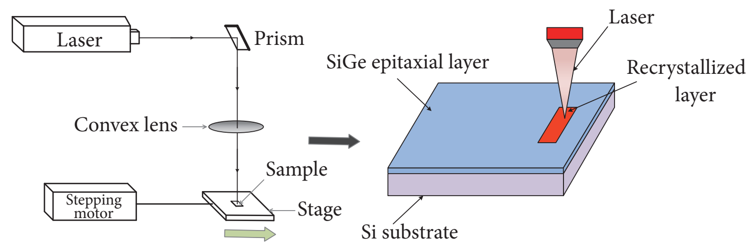

FIGURE 1: Schematic diagram of the laser recrystallization process.

Si substrate is irradiated by the high-energy laser light and rapidly melted and recrystallized by thermal conduction. The TDD of the SiGe epitaxial layer is reduced by the lateral recrystallization process. The vertical proliferation of the threading dislocations in the SiGe epitaxial layer is suppressed, so that the crystal quality of the high-Ge-content SiGe epitaxial layer is significantly improved, which provide another effective approach to obtain high-quality, high-content SiGe epitaxial layer on Si substrate.

Compared with the conventional annealing methods, the laser recrystallization technique has the following advantages: minimized thermal diffusion of the dopants; local selective heating of specific regions, and negligible heating of other parts. In addition, this technique has the advantages of fast, simple process steps and low cost. In view of the application advantages of laser recrystallization in the preparation of high-Ge-content SiGe epitaxial layers, in this paper, a thermal physics model of 808 nm laser recrystallization of high-Ge-content SiGe film (take $Si_{0.2}Ge_{0.8}$ as an example) on Si substrate is established by finite element numerical simulation. The modeling is based on an approach used for Ge/Si system, which is reported in our previous work [9]. Now the approach is modified in this work to consider the high-Ge-content SiGe/Si system instead. Physical model of temperature distribution in $Si_{0.2}Ge_{0.8}$ epitaxial layer is obtained under different laser power, $Si_{0.2}Ge_{0.8}$ epitaxial layer thickness, and initial temperature of epitaxial layer. The obtained results of this paper can provide an important technical support for the laser recrystallization assisted preparation of high-quality high-Ge-content SiGe epitaxial layer on Si substrate.

2. Materials and Methods

In this paper, the multiphysics software COMSOL Multiphysics was used to model and analyze the laser recrystallization process of $Si_{0.2}Ge_{0.8}$ thin film on Si substrate. The temperature distribution of $Si_{0.2}Ge_{0.8}$/Si system under different laser power, different $Si_{0.2}Ge_{0.8}$ layer thickness, and different initial temperatures at 808 nm continuous laser is studied. The obtained results can provide a technical reference for the preparation of high-quality $Si_{0.2}Ge_{0.8}$/Si films for laser recrystallization processes.

The laser heat source used in this paper is a continuous laser with a wavelength of λ=808 nm. The laser is a Gaussian beam along the scanning direction and rectangular shape perpendicular to the scanning direction. The solid heat transfer module was selected in COMSOL Multiphysics to establish a two-dimensional steady state model of $Si_{0.2}Ge_{0.8}$ laser recrystallization on Si. Figure 2 shows the laser recrystallization model of the $Si_{0.2}Ge_{0.8}$/Si system. The numbers indicate the boundaries. The sample absorbs laser energy and performs translational motion along the x-axis.

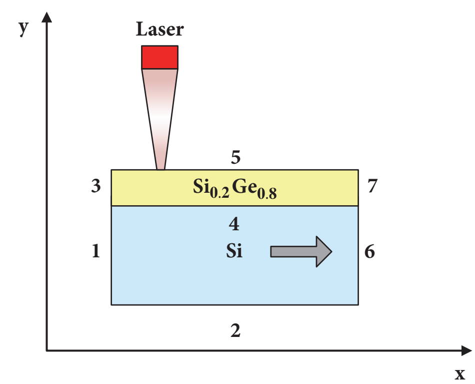

FIGURE 2: The simulated model of the CW laser recrystallization $Si_{0.2}Ge_{0.8}$/Si.

The process of heating a sample by laser follows the general heat equation [10]:

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \nu \nabla T - \nabla (k \nabla T) = Q \quad (1)$$

The irradiation of the laser is simulated by the absorption of laser energy and the temperature change in the sample, where ρ, C_p, k, and v represent the density, heat capacity, thermal conductivity, and translational speed of the sample, respectively. The convection term $\rho C_p \nu \nabla T$ is used to simulate the translational motion of the sample [11]. Since the laser irradiation is continuous and the translational movement speed is constant, the transient change of the laser energy only occurs within a short time from the start of irradiation, so the transient term $\rho C_p(\partial T/\partial t)$ will be ignored. Therefore, the heat equation is the steady state equation. Heat source Q is produced by the absorption of laser energy by the sample, according to the Beer-Lambert law:

$$Q = \frac{2P\alpha}{\pi {r_b}^2} (1 - R) \exp\left(\frac{-2x^2}{{r_b}^2}\right) \exp(-\alpha y) \quad (2)$$

where P, r_b, α, and R are the laser power, the effective laser radius, the absorption coefficient of the material, and the reflectivity of the material surface.

Table 1: Thermal parameters of the materials used for the numerical model [15].

Parameters	Ge	Si	Si_xGe_{1-x}
Melting point T_m [K]	1210	1685	$1210+244x+231x^2$
Density ρ [kg/m^3]	5323	2329	$5323-2495x-499x^2$
Thermal Conductivity k [W/cm*K]	0.6	1.56	$\frac{1}{1.67+48.97x-50x^2}$
Absorption coefficient α [cm^-1]	5×10^4	1×10^3	5×10^4 -4.9×10^4x
Specific heat capacity C_p [J/kg*K]	310	700	c(T)

The main parameters that need to be used in the calculations of (1) and (2) are listed in Table 1. Considering the solid-liquid change of $Si_{0.2}Ge_{0.8}$ epitaxial layer during laser irradiation, the specific heat capacity of $Si_{0.2}Ge_{0.8}$ should be [10]

$$C_p = c(T) = C_{p_{solid}} + \left(C_{p_{liquid}} - C_{p_{solid}}\right) * \text{flc2hs}\left(T - T_m, dT\right) + \frac{L_m}{\sqrt{\pi} * dT} * \exp\left(\frac{-\left(T-T_m\right)^2}{dT^2}\right) \quad (3)$$

where T_m is the melting temperature of the $Si_{0.2}Ge_{0.8}$ epitaxial layer, L_m is the latent heat of phase change, and dT is the half-temperature width of the mushy zone (i.e., the solid-liquid two-phase region), and its value does not normally exceed 5 K. The smooth Heaviside function (flc2hs) in COMSOL is used to describe the abrupt change of temperature and to ensure that the epitaxial layer absorbs heat and changes in the physical properties during the phase transition [12]. Two solid-liquid phase transitions are considered during the laser recrystallization of the $Si_{0.2}Ge_{0.8}$ epitaxial layer. The first phase transition occurs when the absorption energy of the laser energy in the epitaxial layer is transformed into the latent heat of phase change, L_m, and the temperature increases. When the temperature of the epitaxial layer reaches the melting point, the solid state changes to the liquid state; the second phase change occurs after the laser irradiation stops. The temperature of the epitaxial layer of $Si_{0.2}Ge_{0.8}$ decreases, and when the temperature reaches the melting point again, the epitaxial layer releases heat. The process of lateral recrystallization occurs. It changes from a liquid state to a solid state again.

COMSOL Multiphysics used the finite element method to solve nonlinear partial differential equations to simulate the laser recrystallization process of $Si_{0.2}Ge_{0.8}$/Si system. Finite element method is a commonly used high-efficiency numerical calculation method. Its principle is to divide the continuous solution domain into a discrete group of unit assemblies and use the hypothesized approximate function in each cell to represent the unknown field function to be solved in the solution domain, so that a continuous infinite degree of freedom problem becomes a discrete finite degree of freedom problem. In the finite element method, optimizing the mesh is very important for obtaining accurate numerical solutions. The number and form of the grids will directly affect the calculation accuracy and the calculation scale. If the number of grids is too small, the calculation results will be inaccurate or the results will not converge, resulting in the inability to obtain ideal results. If the number of grids is too large, it will take a lot of time to make the calculation scale larger, and the calculation efficiency will be low [13]. There are many factors to consider when meshing and optimizing meshes, such as the number of meshes, mesh density, mesh boundaries, and demarcation points. Since the $Si_{0.2}Ge_{0.8}$ epitaxial layer has a high absorption coefficient and we need to study the temperature change in the epitaxial layer, therefore the mesh of the $Si_{0.2}Ge_{0.8}$ epitaxial region needs to be refined to satisfy the rapid spatial change of the absorbed laser power, so that a more accurate numerical solution can be obtained. A coarse mash is employed for the Si substrate area to improve the calculation efficiency. The refined $Si_{0.2}Ge_{0.8}$/Si system grid is shown in Figure 3. It can be clearly seen from the figure that the epitaxial layer grid is denser than the substrate grid.

Appropriate boundary conditions are crucial for obtaining accurate numerical solutions. Figure 2 shows the various boundaries of the $Si_{0.2}Ge_{0.8}$/Si model. For the boundaries 1, 2, and 3, the Dirichlet condition holds; i.e., the temperature T is set to a fixed temperature value T_0. The adiabatic condition is applied to the $Si_{0.2}Ge_{0.8}$/Si interface (boundary 4), and the heat flux is specified to 0 to allow the continuity of the thermal field [10]:

$$\mathbf{n} \cdot \left(k_{Si_{0.2}Ge_{0.8}} \nabla T\right) = \mathbf{n} \cdot \left(k_{Si} \nabla T\right) = 0 \quad (4)$$

where n is the outer normal direction vector of the surface and k is the thermal conductivity.

Convection and radiative heat transfer occur at the sides of the upper surface and sample translational motion (boundaries 5, 6, and 7), causing heat loss [14]:

$$\mathbf{n} \cdot (k\nabla T) = h\left(T_{inf} - T\right) + \sigma\varepsilon\left(T_{amb}^4 - T^4\right) \quad (5)$$

where h is the convective heat transfer coefficient, T_{inf} is the external temperature, σ is the Stefan-Boltzmann constant, ε is the surface emissivity, and T_{amb} is the ambient temperature. $h(T_{inf} - T)$ represents the heat flux generated by convection heat transfer, and $\varepsilon\sigma(T_{amb}^4 - T^4)$ represents the heat flux generated by radiative heat transfer.

3. Results and Discussion

In the process of laser recrystallization, the parameters of the incident laser and the properties of the sample are two factors that affect the quality of the recrystallized film, including the incident laser output power, epitaxial layer thickness,

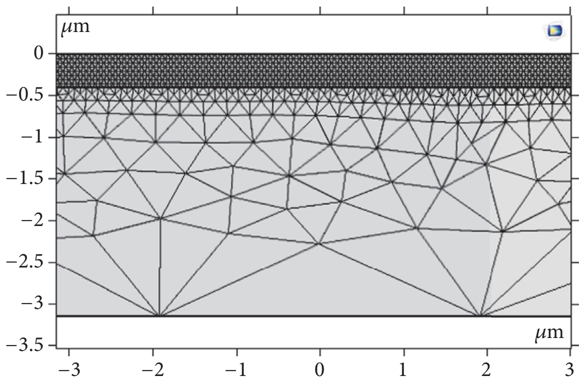

FIGURE 3: The refined mesh for $Si_{0.2}Ge_{0.8}$/Si.

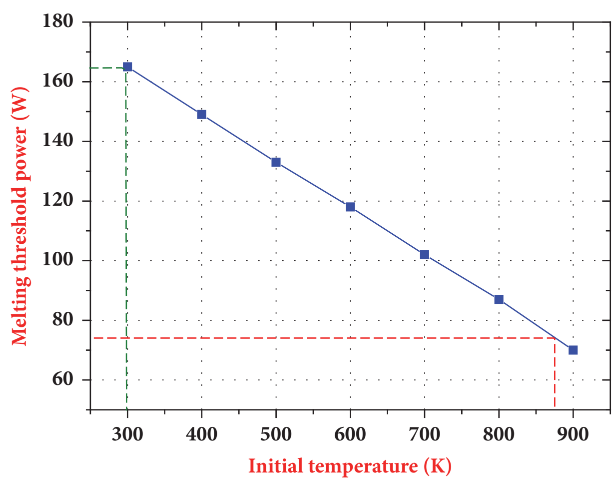

FIGURE 4: The melting threshold power of Ge under different initial temperatures.

and the initial temperature of the sample. By changing these parameters and studying the temperature distribution of the $Si_{0.2}Ge_{0.8}$/Si system, the laser recrystallization process can be optimized. The laser recrystallization technique with optimal process parameters provides theoretical guidance for the preparation of high-quality $Si_{0.2}Ge_{0.8}$ epitaxial films.

Figure 4 shows the melting threshold power required for the recrystallization of 400 nm thick $Si_{0.2}Ge_{0.8}$ film on a Si substrate at different initial temperatures. It can be seen from the figure that as the initial temperature increases, the power required for laser recrystallization of the system decreases linearly. The power required for the laser recrystallization of the system at 300 K at room temperature is 165 W, while the power required at 873 K is only about 74 W. Therefore, choosing a reasonable initial preheating temperature can effectively reduce the laser recrystallization power of $Si_{0.2}Ge_{0.8}$/Si system, which is beneficial to the control of process cost.

There is an important reason why the initial preheating is needed before the $Si_{0.2}Ge_{0.8}$/Si system is recrystallized. The laser recrystallization is a heat treatment process. If the laser recrystallization is performed directly without preheating the sample, the temperature gradient within the $Si_{0.2}Ge_{0.8}$/Si system will be steep during the recrystallization temperature rising process and the cooling process after laser irradiation, which is unfavorable to the crystal quality of the epitaxial layer and may even cause cracking phenomenon [16].

Based on the above two points, the preheating process is essential before laser recrystallization of $Si_{0.2}Ge_{0.8}$/Si system. Considering the two factors of process cost control and recrystallizing quality effect, combined with our experience in the traditional heat treatment of $Si_{0.2}Ge_{0.8}$/Si system and the simulation results in Figure 4, we propose using 873 K as the preheating temperature of the $Si_{0.2}Ge_{0.8}$/Si system before laser recrystallization.

The thickness of the $Si_{0.2}Ge_{0.8}$ epitaxial layer is also an important parameter that needs to be considered in the laser recrystallization of the system. When the sample is illuminated by the laser, part of the laser energy is reflected, the other part is absorbed, and the rest is transmitted. The absorption rate is the fraction of absorbed laser light. The 808 nm laser absorption rate is different for different epitaxial layer thicknesses. The laser recrystallization energy should be absorbed by the $Si_{0.2}Ge_{0.8}$ epitaxial layer as much as possible to ensure the melting effect. Figure 5 shows the schematic diagram of the laser reflection, absorption, transmission, and the FDTD simulation results of the absorption rate of 808 nm laser in $Si_{0.2}Ge_{0.8}$ epitaxial layer and Si substrate under different epitaxial layer thickness conditions. It can be seen from the figure that when the epitaxial layer thickness of $Si_{0.2}Ge_{0.8}$ reaches 300 nm or more, the absorption rate of the 808 nm laser in the epitaxial layer exceeds 50%. Moreover, as the thickness of the $Si_{0.2}Ge_{0.8}$ epitaxial layer increases, the absorptivity of the 808 nm laser in the epitaxial layer will further increase. Therefore, in this paper, $Si_{0.2}Ge_{0.8}$ epitaxial layer thickness must reach at least 300 nm in the laser recrystallization process of $Si_{0.2}Ge_{0.8}$/Si system.

Another issue is also worthy of attention. Is the thickness of the $Si_{0.2}Ge_{0.8}$ epitaxial layer thicker the better? If the $Si_{0.2}Ge_{0.8}$ epitaxial layer is too thick, although the absorption rate of the 808 nm laser in the epitaxial layer can be further increased, the temperature difference between the upper and lower layers of the $Si_{0.2}Ge_{0.8}$ epitaxial layer is large, and the full $Si_{0.2}Ge_{0.8}$ epitaxial layer cannot be melted and recrystallized. To achieve melting and recrystallization of the whole $Si_{0.2}Ge_{0.8}$ epitaxial layers, laser power needs to be further increased (see Figure 6).

Considering comprehensively, this paper proposes choosing 300 nm~400 nm as the thickness of $Si_{0.2}Ge_{0.8}$ epitaxial layer in laser recrystallization of Si0.2Ge0.8/Si system.

The following further discusses the selection of laser power parameters in the laser recrystallization process. It is known from the foregoing discussion that the laser power is relevant in the selection of two important parameters of the thickness of the epitaxial layer of $Si_{0.2}Ge_{0.8}$ and the preheating temperature. The focus of the laser power parameter discussion here is to study the epitaxial layer thickness (400 nm) and the preheating temperature (873K) of the $Si_{0.2}Ge_{0.8}$ layer that has been determined in this paper. The temperature distribution and the temperature of the upper and lower surfaces of the $Si_{0.2}Ge_{0.8}$ epitaxial layer at different laser powers are examined. According to the temperature values of the upper and lower surfaces of the $Si_{0.2}Ge_{0.8}$ epitaxial layer,

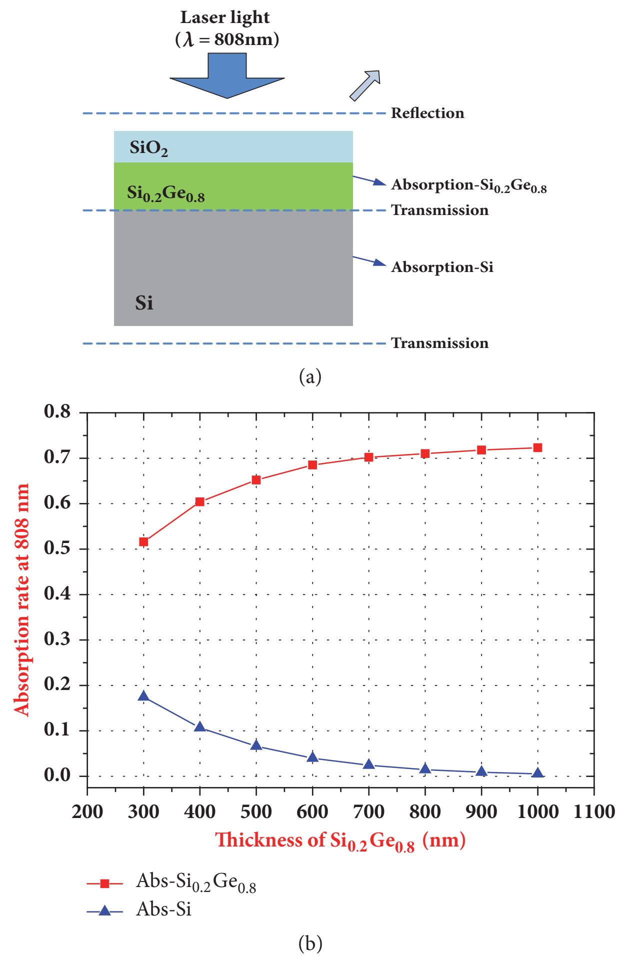

FIGURE 5: (a) Schematic diagram of the laser reflection, absorption, and transmission (here the SiO2 capping layer is used here to protect the Ge film from damage). (b) Absorption rates at λ=808 nm of $Si_{0.2}Ge_{0.8}$ and Si layer as a function of $Si_{0.2}Ge_{0.8}$ thicknesses.

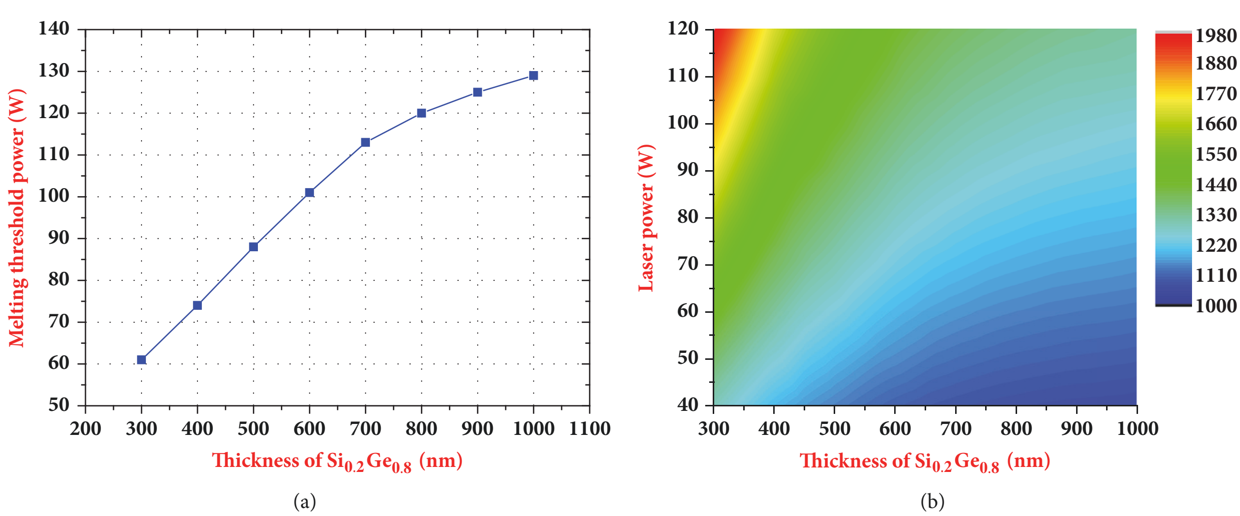

FIGURE 6: (a) Melting threshold power as a function of $Si_{0.2}Ge_{0.8}$ thicknesses at 873 K. (b) Peak temperature at the surface of $Si_{0.2}Ge_{0.8}$ layer simulated using a range of laser powers and $Si_{0.2}Ge_{0.8}$ thicknesses.

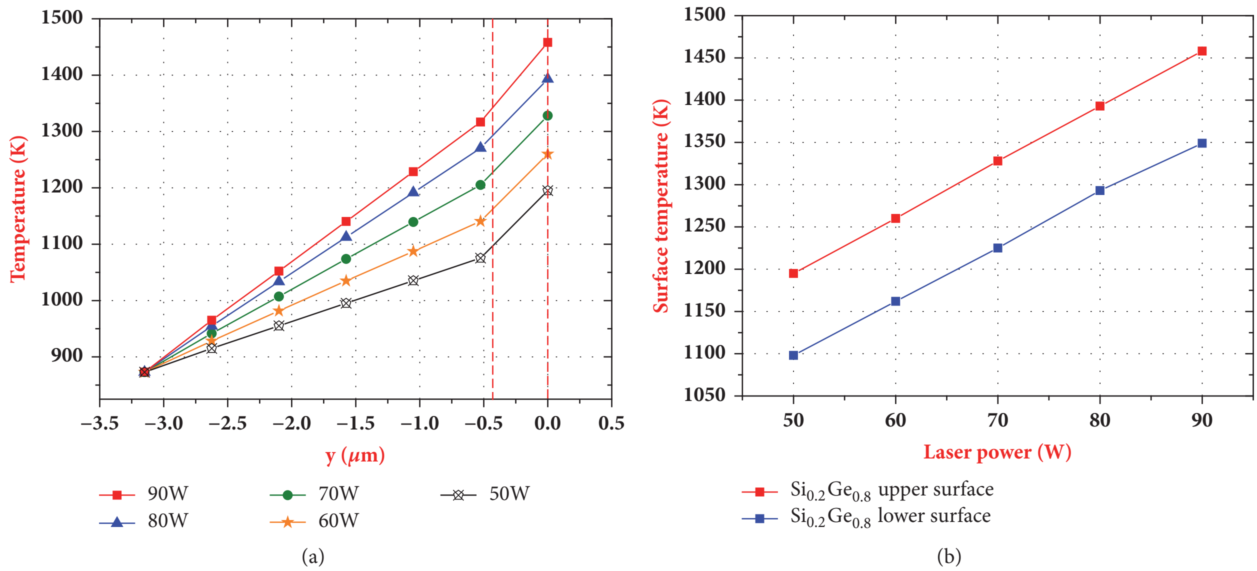

FIGURE 7: (a) Longitudinal temperature changes of the sample at x = 0 with different laser powers. The vertical lines delimit the area of $Si_{0.2}Ge_{0.8}$ layer. (b) Peak temperatures of $Si_{0.2}Ge_{0.8}$ upper surface and lower surface as a function of laser power.

it is determined whether the $Si_{0.2}Ge_{0.8}$ epitaxial layer is fully melted to determine the optimal laser power parameter.

Figure 7 shows the simulation results of the internal temperature of $Si_{0.2}Ge_{0.8}$ epitaxial layer/Si substrate and the peak temperatures of $Si_{0.2}Ge_{0.8}$ upper surface and lower surface under different power. The preheating temperature is 873 K and the thickness of the $Si_{0.2}Ge_{0.8}$ epitaxial layer is 400 nm. As can be seen from the figure, the $Si_{0.2}Ge_{0.8}$/Si sample temperature gradually increases as the incident laser power increases. From the surface of the sample to the inside of the sample, the temperature gradually decreases. The incident laser energy is absorbed by the $Si_{0.2}Ge_{0.8}$/Si sample after heat conduction and the temperature of the sample increases. When the laser power reaches 70W, the upper surface of the $Si_{0.2}Ge_{0.8}$ epitaxial layer has melted (the melting point of $Si_{0.2}Ge_{0.8}$ is 1268 K). The lower surface is also close to melting; when the laser power is 80 W, the upper and lower surfaces of the $Si_{0.2}Ge_{0.8}$ epitaxial layer have exceeded the melting point, indicating that the $Si_{0.2}Ge_{0.8}$ epitaxial layer achieves full melting. Therefore, it is suggested that the incident power between 70 W and 80 W is selected as the laser recrystallization power of the $Si_{0.2}Ge_{0.8}$/Si system.

Based on the above simulation results of the incident laser output power, epitaxial layer thickness, and sample initial temperature, the proposed laser recrystallization process parameters for the $Si_{0.2}Ge_{0.8}$/Si substrate system are as follows: System 873 K preheating, $Si_{0.2}Ge_{0.8}$ epitaxial layer 400 nm thick, and 808 nm laser power 74 W. Figure 8 shows the COMSOL Multiphysics simulation results using the laser recrystallization process parameters $Si_{0.2}Ge_{0.8}$/Si substrate system. Figure 9 shows the surface temperature distribution of $Si_{0.2}Ge_{0.8}$ and the longitudinal temperature distribution of the $Si_{0.2}Ge_{0.8}$/Si substrate system at x = 0. It can be seen from the figure that the maximum temperature of the $Si_{0.2}Ge_{0.8}$/Si sample reaches 1352 K, which exceeds the melting point of $Si_{0.2}Ge_{0.8}$, indicating that the epitaxial layer has melted. It can be clearly seen from Figure 8 that the laser heating area is in the shape of a droplet. The temperature of the sample is highest at the center of the heating area of the laser beam. The laser energy passes through the heat conduction, and the temperature gradually decreases from the surface of the sample to the inside of the sample. When the laser energy reaches the Si substrate, it is already very weak, so that the Si substrate does not melt, thereby realizing the laser recrystallization of the $Si_{0.2}Ge_{0.8}$ epitaxial layer without damaging the substrate material.

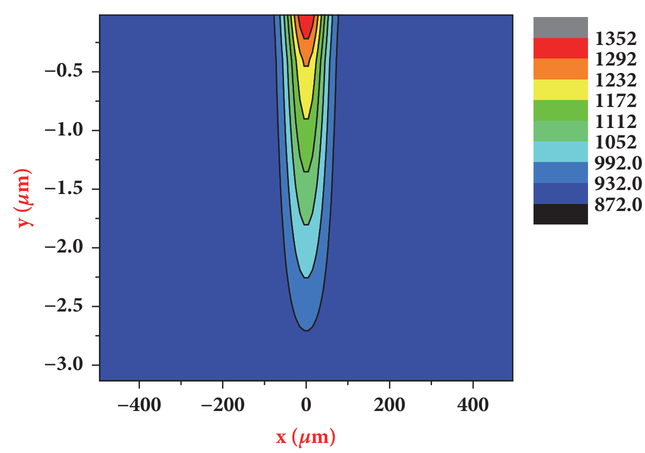

FIGURE 8: Temperature distribution of the $Si_{0.2}Ge_{0.8}$/Si virtual substrate simulated by COMSOL Multiphysics.

4. Conclusion

In this paper, a thermal physics model of continuous wave laser recrystallization of high-Ge-Content SiGe (for example,

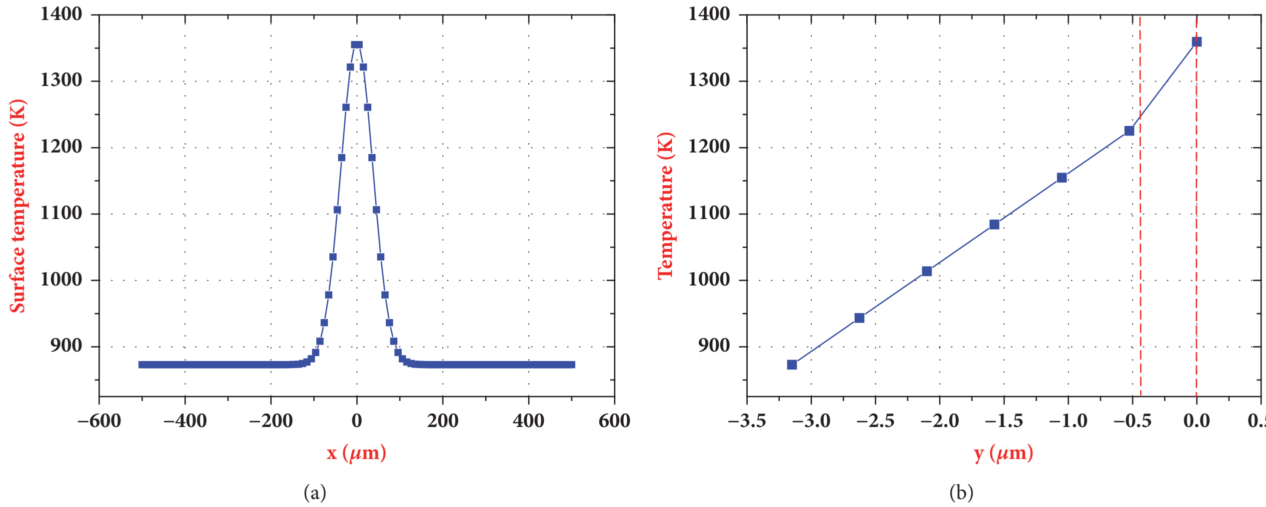

Figure 9: (a) Evolution of the temperature at the surface of $Si_{0.2}Ge_{0.8}$ layer in the scan direction x and (b) longitudinal temperature changes of the sample at x = 0. The vertical lines delimit the area of $Si_{0.2}Ge_{0.8}$ layer.

$Si_{0.2}Ge_{0.8}$) on Si substrate was established using COMSOL Multiphysics finite element analysis software. The effects of different laser and material parameters on the temperature distribution of $Si_{0.2}Ge_{0.8}$/Si substrate system were simulated in detail, and the optimum process parameters for laser recrystallization of $Si_{0.2}Ge_{0.8}$/Si substrate system were determined. The numerical simulation results show that the preheating treatment before laser recrystallization in $Si_{0.2}Ge_{0.8}$/Si system can not only avoid the material damage caused by the large temperature gradients but also reduce the process cost. The thickness of $Si_{0.2}Ge_{0.8}$ epitaxial layer affects the laser absorption rate. Selection of a reasonable epitaxial layer thickness is possible to realize the melting and recrystallization of the whole $Si_{0.2}Ge_{0.8}$ epitaxial layer. The temperature of the $Si_{0.2}Ge_{0.8}$/Si substrate system increases as the incident laser power increases. Based on the simulation results of the incident laser output power, the thickness of the epitaxial layer, and the initial temperature of the sample, the proposed laser recrystallization process parameters for the $Si_{0.2}Ge_{0.8}$/Si substrate system are as follows: 873 K preheating, $Si_{0.2}Ge_{0.8}$ epitaxial layer 400 nm thick, and 808 nm laser power 74 W. The process of laser recrystallization can be optimized through reasonable selection of process parameters, which will provide theoretical guidance for the preparation of high-quality $Si_{0.2}Ge_{0.8}$ epitaxial films.

Data Availability

The table and graphic data used to support the findings of this study are included within the article. All data of this paper used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

Acknowledgments

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