Proceedings of the 4th International Conference on Mathematical Physics and Computational Simulation
DOI: 10.54254/2753-8818/2026.35094

Si-Ge-Sn Alloys for Infrared Optoelectronic Devices

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Abstract. Silicon photonic device has compatibility property with CMOS technique; however, it is restricted by the non-direct bandgap of silicon, which brings about bad light emission efficiency and a disability to detect light with wavelengths that surpass 1.1 µm. Germanium makes the detection scope become wider toward the short-wave infrared area. Even so, its indirect bandgap still brings a barrier to the development of high-efficiency luminescence devices. Si-Ge-Sn alloys have become the foreground as a hopeful solution because the adding of tin can bring out a direct bandgap changing. The band gap of these alloy materials can be regulated in the interval from 0 to 0.8 eV, which covers the short-wave to mid-wave infrared spectral range. This review makes a summary of current research progresses about Si-Ge-Sn alloys which are used for infrared optoelectronic devices. It concentrates tightly on four key domains: theoretical energy band construction, material epitaxial growth, device utilizations, and important difficulties. Worthy achievements that attract attention include direct-bandgap Ge-Sn light-emitting lasers, middle-infrared light detecting devices, and the first-time on-chip integration work. The still existing questions, for example tin separation, heat stability, ohmic contact points, and restrictions of the CMOS heat budget, are discussed deeply, together with the future research directions. Defeating these difficulties will let out the whole capability of Si-Ge-Sn compound materials for low-cost, high-effectiveness infrared optoelectronic devices which are totally integrated on the silicon base platform.

Keywords: Si-Ge-Sn alloys, Direct bandgap, Infrared optoelectronics, Ge-Sn lasers

1. Introduction

Silicon photonics has become a main selection for the making of photonic integration devices, therefore it is largely because of the matching degree of its produce flow with CMOS technology. But there is a big problem that has relation to the Si material. Its indirect bandgap characteristics bring about extremely low luminous efficiency, and Si is nearly transparent to the light which has wavelengths longer than 1.1 µm. These characteristics bring difficulty to the fabrication of high-efficiency light-emitting devices on Si-based platforms and the detection of infrared light. Although the adding of Ge can broaden the detection scope to the short-wave infrared area, Ge also possesses an indirect bandgap, this therefore hinders the development of an effective light-emitting source.

For solving these restriction conditions, research workers have produced an interest in Si-Ge-Sn alloy materials. Putting Sn into the alloy is able to change the originally indirect bandgap structure into a direct bandgap, hence opening the possibility for making light-emitting sources with Si-based materials. The bandgap of this alloy may be stably adjusted in the interval from 0 to 0.8 eV, hence it covers the short-wave to mid-wave infrared spectrum region. From the time when Soref and his work partners theoretically forecasted a direct-bandgap change in Si-Ge-Sn alloys in the 1990s, and along with the progress of non-equilibrium epitaxy techniques such as molecular beam epitaxy (MBE) and chemical vapor deposition (CVD), very much advance has been obtained in the preparation and device application of this material system [1]. The present research carries out an evaluation on the current situation of researches which are about Si-Ge-Sn alloys that are applied in infrared optoelectronic devices.

2. Theoretical foundation and material preparation

2.1. Mechanisms of band structure engineering

2.1.1. Band crossing and the realization of direct bandgap

The energy band arrangement of Si-Ge-Sn alloy materials is mainly controlled by the relative positions of the Γ valley, L valley, and X valley. Along with the increment of Sn's proportion inside the alloy, the energy of the Γ valley undergoes a drop that has a notably rapid speed. Speak particularly, inside $Ge_{1-x}Sn_x$, when perfect no-strain conditions are satisfied, a Γ - L cross-over will have occurrence when the Sn content reach 8–10%. On this juncture, the energy of the Γ valley becomes lower than that of the L valley, hence it makes the material become a direct-bandgap one. Nevertheless, even inside direct-bandgap alloy materials, a part of charge carriers still remain in the indirect (L and X) energy valleys under room temperature on account of thermal excitation. This therefore brings about a reduction in the radiative recombination efficiency, and hence it still remains a limiting factor for the present performance of devices. Furthermore, the composition undulations and partial stress changes also have a comparatively notable effect on the crossing point.

The sketchy energy band structure of Si-Ge-Sn alloys, which is shown in Figure 1, is drawn as a function that relates to the Sn component content. It gives display to the relative energy magnitudes of the Γ, L, and X valleys. Furthermore, the position of direct-bandgap transformation is clearly indicated.

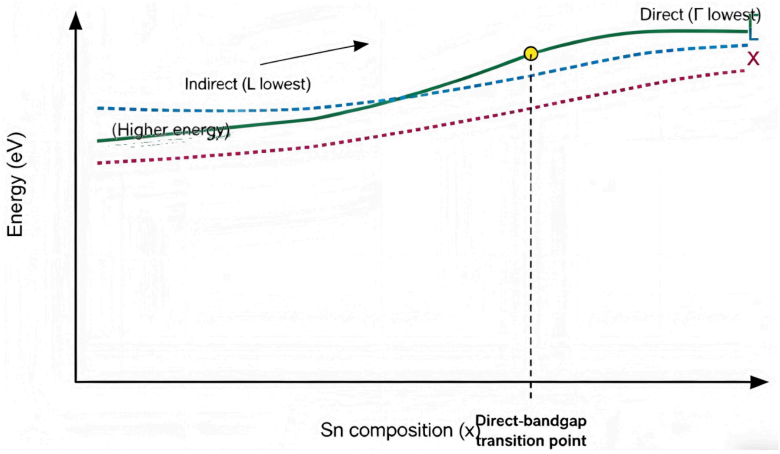

Figure 1. Schematic band structure of Si-Ge-Sn alloys as a function of Sn composition

2.1.2. Effect of strain engineering on band structure

In the field of heterostructure materials, silicon (Si), germanium (Ge), tin (Sn) have obvious differences in their lattice parameters. This difference causes that quite big inner stress is brought into the inside of the material. The crystal lattice mismatch that exists between alpha-tin (α-Sn) and germanium is about 15 percent. By way of comparison, the lattice mismatch between α - Sn and silicon is still larger, reaching 20%. This non-consistency therefore leads to the existence of biaxial or uniaxial stress inside the material. On another hand, the biaxial tensile strain possesses the effect of decreasing the direct band gap energy. It also makes the Γ valley get a lower position when compared with the valence band maximum. As the result, radiative combination has been increased. By opposite way, biaxial press strain possesses an opposite effect. It widens the direct band gap and raises the Γ valley, which is not good for the light emission. Pulling strain further makes the energy gap smaller, therefore it makes the detection cut-off wavelength move toward the direction of bigger numerical values. The strain's character and scope can be adjusted through the careful selection of appropriate base materials and buffer layers.

2.2. Material epitaxial growth and defect control

2.2.1. Comparison of MBE and CVD techniques

In the condition of solid state, the solubility degree of α-tin (α-Sn) inside germanium (Ge) and also silicon (Si) is extremely small, and it drops lower than one atomic percent. Therefore, non-balance growth methods are necessary for the preparation of silicon-germanium-tin (Si-Ge-Sn) alloys. Molecular beam epitaxy (MBE) is often used because it can give careful control of the alloy's component and the boundary faces between different layers. This method especially is suitable for carrying out deep explorations on the properties of materials. However, the MBE method has the own inherent disadvantages which are contained in it. It possesses a comparatively slow growth speed and therefore brings high expenses for the equipment. On another hand, the chemistry vapor deposit (CVD), in particular the depressurization chemistry vapor deposit (RP-CVD), therefore displays more appropriate compatibleness for other manufacture procedures. By means of the employment of RP-CVD, Si-Ge-Sn alloys which have tin inside can be fabricated with a tin content that reaches as high as 15–20%.

2.2.2. Compositional inhomogeneity and strain relaxation

The effect which temperature and growth speed exert on the position-occupying introduction of Sn has been studied by the authors. When temperature is relatively low (for example, below 350 °C), and this is matched with an appropriate growing speed, therefore, the segregation of Sn and compositional non-uniformity can be greatly decreased. In addition, the lattice mismatch causes the generation of stress, which can be accumulated slowly. This piling up can bring about dislocations and lattice relaxation, therefore it brings a negative influence to the optoelectronic properties of the material [1].

2.2.3. Impact of buffer layer design on crystal quality

The designing of the buffer layer has very important meaning in easing problems which are connected with material mismatch. The research team of Bauer used a GeSn buffer layer which was placed on a Si (100) substrate for obtaining high-quality Si-Ge-Sn ternary alloys [2]. This buffer layer has the function of absorbing the strain difference which exists between the substrate and the epitaxial layer. In addition, other structures such as composition-gradient buffer layers, low-temperature Ge buffer layers, and SiGe virtual substrates can also scatter stress. Therefore, the number of defects that exist in the uppermost layer of active material is much smaller.

3. Advances in Si-Ge-Sn based infrared optoelectronic devices

3.1. Infrared photodetectors

The silicon-germanium-tin alloys enable the light detection range to be widened from short-wave infrared to mid-wave infrared. After the Sn content exceed 10 percent, this material displays direct-bandgap characteristics and keeps strong absorbing action that goes past the 1.8 μm cut-off position of Ge. The research group of Zhou directly made GeSn/SiGeSn heterojunction photoelectric detectors on Si wafers, and realized mid-infrared detection. Through the utilization of RP-CVD when the Sn content lies in the range from 15% to 20%, the absorption edge has been extended to exceed 3.75 μm [3]. One long-existing problem is that whether atomic displacements can produce an influence on the dark current. Even so, it has already been demonstrated by research that optimized compositionally graded buffer layers are able to effectively reduce the defect density [1, 3].

3.2. Infrared light sources and lasers

In year 2015, Wirths and his work companions put forward the first optically excited GeSn laser which was on a silicon substrate [4]. The active layer which is made of GeSn possesses a tin content that is approximately 12–16%. This magnitude was sufficient for achieving the direct bandgap. Under ideal situations, the theoretical Γ-L crossing change occurs at 8–10%, yet in actual devices, a larger tin content is often needed on account of strain and defects [4]. At a later time, microcavity laser devices which have a wavelength of 3 μm were successfully developed. These laser devices employed SiGeSn/GeSn heterogeneous structures for strengthening carrier restriction [5]. Nevertheless, the electricity-driven GeSn lasers at the present time can only work under very very low temperature conditions. The primary causes for this circumstance are the inadequate conduction band offset and elevated optical losses [1, 3].

3.3. On-chip integration and modulator devices

To the photonic integrated circuits which are called PICs for short, monolithic integration has the highest importance. A GeSn light-detector that is integrated with a Si waveguide has achieved a responsivity which is larger than 0.3 A/W at 2 μm [3]. But the modulation bandwidth is kept below 1 GHz. This main reason therefore is the low carrier mobility and high contact resistance [1]. For the solving of this problem, researchers have caused Si-Ge-Sn materials to combine with Ge or SiGe virtual substrates for the effective control of material defects [2].

4. Key challenges and optimization strategies

4.1. Material quality and thermal stability

The dissolving capacity of tin (Sn) inside germanium (Ge) and silicon (Si) is extremely small, being lower than 1 atomic percent. For the prevention of the segregation of tin, it is a necessary thing that non-equilibrium growth be conducted at temperatures which are lower than 350 °C, which is what references [1, 6] have pointed out. But, when temperature becomes higher, for example when people process devices, tin has the tendency that it can generate precipitates. At the same time, the inner stress that exists inside the material gets relaxed, hence this leads to a decrease of the quality of the material. For solving this problem, many kinds of methods have been proposed by researchers. These contain the usage of a low-temperature germanium buffer layer, a buffer layer which has a composition that changes in a grading way, or a silicon-germanium (SiGe) virtual substrate, as what references cite [2, 7, 8].

4.2. Metal–semiconductor contact and carrier transport

Because the GeSn has narrow bandgap, therefore the Fermi level is fixed near the valence band, this makes obtaining n-type ohmic contacts have very big challenge. Furthermore, a type-II band arrangement is built between GeSn and SiGeSn, hence it causes asymmetrical carrier movement. In the actual devices of the real world, for example detectors, this therefore causes a comparatively high dark current. In the laser devices, this factor has an influence upon the efficiency of carrier injection. Proposed solutions include the employment of a heavily doped middle layer, the optimization of blocking layer components, or the usage of surface passivation by Al_2O_3 [1, 7].

4.3. Compatibility with CMOS process flow

The carrying out of processing under low temperature conditions, that is to say temperature values lower than 450 °C, is not able to be matched with the traditional high-temperature working procedures which take place above 900 °C. Among all semiconductor materials, tin (Sn) possesses a very high diffusion velocity, and therefore it can easily bring about pollution problems. For getting over these difficulties, many methods can be used by people. These contain the back-end-of-line (BEOL) integration work, laser heat treatment, and the utilization of diffusion blocking layers such as titanium nitride (TiN) and tantalum nitride (TaN) [1].

5. Conclusion

This evaluation has researched Si-Ge-Sn alloys, which is a special group-IV material system that can achieve a direct bandgap. The energy value of the bandgap may be adjusted between 0 and 0.8 electron-volts, and it covers the spectral range from short-wave infrared to mid-wave infrared. Through changing the alloy component and using various deformations, the crossing place of the Γ and L valleys may be adjusted. Two main preparation methods are existed: molecular beam epitaxy (MBE) and decompression chemical vapor deposition (RP-CVD). These methodologies have successfully been utilized by researchers to prepare Si-Ge-Sn alloy thin films that possess a tin (Sn) component content which reaches as high as 20%. Outstanding achievements inside this domain include extremely sensitive mid-infrared light detecting devices, optical pumping light generators, and the first steps which are on the road to monolithic combination.

The results of this examination show that alloys which are constituted by silicon (Si), germanium (Ge), and tin (Sn) possess great potential for infrared optoelectronic devices which are constructed on silicon-based platforms. This circumstance is especially the case for application scenarios in which it is necessary to overcome the restrictions that are connected with the indirect bandgap of silicon and germanium. Even so, there exist a number of key difficulties that still require people to solve them. These include the separation of tin, the low heat stability, the hardship of building ohmic contacts, issues with energy band matching, and the limitations on the heat budget brought by complementary metal-oxide-semiconductor (CMOS) processes.

The main contribution of this review is in comprehensively summing up the current understanding and pointing out the key difficulties in the development of Si-Ge-Sn alloys. This is beneficial for scientific workers who want to design the next-generation group-IV infrared apparatuses, therefore it clarifies the connections among component, stress, energy band arrangement, and apparatus working performance.

In later research works, people should put focus on getting an electrically pumped continuous-wave laser, which runs under room temperature through employing group-IV materials. The research objects include strengthened light limiting action, more useful n-type doping and linking work, and the usage of Si-Ge-Sn blocking layers which have bigger band gaps. Photonic integrated circuits which are built upon Si-Ge-Sn, they are especially very suitable for mid-infrared sensing work. Through the combination of active devices and passive Si/Ge components, it is therefore possible that low-cost, high-performance spectroscopic systems can be created. Besides, the combination of two-dimensional materials (for example graphene) with group-IV alloys has the possibility to raise photoresponse and reduce dark current.

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