Photovoltaic Characterization of $Si_{1-x-y}Ge_xSn_y$ Ternary Alloy as Versatile Absorber Material for Group-IV Solar Cells

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***Abstract*– The structure of semiconductor alloys is critical in the tailoring of their optoelectronic properties to ensure high-performance photovoltaic (PV) use. In the work presented here, we explore Group IV $Si_{1-x-y}Ge_ySn_x$ ternary alloys with a constant content of 14% Sn and different Ge concentrations for potential use as absorber layers in solar cells. According to simulation data, increasing the Ge concentration results in a systematic decrease in the bandgap, which redshifts the external quantum efficiency (EQE) and boosts absorption in the near-infrared.**

Index terms – SiGeSn alloy, NIR region, EQE, Integrated J_{SC}.

I. INTRODUCTION

The advancement of photonic technologies owes much to Group IV elements e.g., Si, Ge, Sn—and their semiconductor alloys due to their widespread availability, CMOS compatibility, and tunable electronic properties. Si, the most extensively used semiconductor and cornerstone of integrated photonic circuits, offers mature processing infrastructure and cost-effective fabrication. Although the indirect bandgap of Si limits its efficiency in photon absorption and carrier generation, Si excels in passive photonic components such as waveguides, modulators, and photodetectors [1]. Ge, with its narrower bandgap and higher carrier mobility, is particularly useful in near-infrared (NIR) photodetection and as a complementary material to Si in heterojunction photodetectors and plasmonic structures. Furthermore, the incorporation of Sn into SiGe matrices to form SiGeSn ternary alloys has further expanded the application landscape by enabling direct bandgap behavior at specific compositions of Sn in the alloy, particularly at high Sn content. This breakthrough opens the possibility of integrating efficient group-IV-based PV devices on Si platforms, overcoming the long-standing limitations of indirect bandgap emission in conventional Si and Ge [2]. Among various semiconductor alloys under research, Group IV ternary $Si_{1-x-y}Ge_ySn_x$ can showcase potential as a tunable and stable material for PV devices in next-generation PV systems. Varying the Ge and Sn composition enables precise control across the bandgap in the desirable range. This work showcases the potential of alloy $Si_{1-x-y}Ge_ySn_x$ as an absorber layer. The bandgap of the ternary alloy has been calculated using Vegard's law [3].

$$E_g\left(Si_{(1-x-y)}Ge_ySn_x\right) = (1-x-y)E_g^{\Gamma}(Si) + yE_g^{\Gamma}(Ge) + xE_g^{\Gamma}(Sn) - b_{\Gamma}^{SiGe}y(1-x-y) - b_{\Gamma}^{SiSn}x(1-x-y) - b_{\Gamma}^{GeSn}xy \quad (1)$$

Where E_g represents the bandgap of the particular element, and b represents the bowing parameter.

Table I. Energy bandgap and bowing parameters for Si, Ge, and Sn

Valley	E_g(Si) eV	E_g(Ge) eV	E_g(Sn) eV	b_{SiGe} eV	b_{SiSn} eV	b_{GeSn} eV
L	2	0.66	0.14	0	0 1	0.91
Γ	4.06	0.795	-0.413	0.21	13.2	2.1

II. DEVICE STRUCTURE AND COMPUTATIONAL METHODOLOGY

The basic device architecture of a PV device consists of an absorber layer is the core responsible for absorbing photons and converting them to charge carriers. Between the Electron and the Hole transport layer ((ETL, HTL) a Absorber layer is positioned to efficiently capture photons and generate charge carriers. ETL and HTL are responsible for transporting the photogenerated charge carriers to the respective electrodes, i.e., right contact and front contact [4]. The proposed device structure incorporates FTO as a transparent oxide layer to minimize the reflectivity of incoming light and enhance light absorption. WS_2 (50nm) is incorporated as an ETL, $Si_{1-x-y}Ge_ySn_x$ (1000nm) is incorporated as an absorber layer, and Cu_2O (50nm) is used as an HTL. The device is simulated using software SCAPS-1D[5]. The simulation is performed at an ambient temperature of 300K using an AM 1.5G sun spectrum.

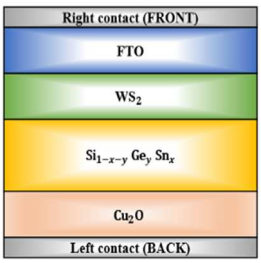

Fig.1. Proposed device structure FTO/WS_2/$Si_{1-x-y}Ge_ySn_x$ /Cu_2O with group IV $Si_{1-x-y}Ge_ySn_x$ as an absorber layer, AM 1.5G has been used as the illumination spectrum in simulation.

III. RESULTS AND DISCUSSION

The J-V response of the designed device structure FTO/WS_2/$Si_{1-x-y}Ge_ySn_x$ /Cu_2O for different Ge compositions y = 0.25, 0.30, 0.35,0.40 at fixed Sn composition x = 0.14. Figure 2 represents that as the Ge composition increasing the J_{SC} increases. This increase in J_{SC} is due to decrease in bandgap which allows more photons to get absorbed in $Si_{0.46}Ge_{0.40}Sn_{0.14}$.

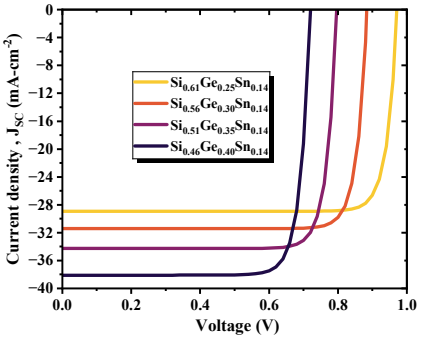

Fig.2. J-V characteristics for proposed device structure FTO/WS_2/$Si_{1-x-y}Ge_ySn_x$ /Cu_2O.

Figure 3 shows that as the Ge composition is increasing in the alloy $Si_{1-x-y}Ge_ySn_x$ from 0.25 to 0.40 the EQE curve for the proposed device FTO/WS_2/$Si_{1-x-y}Ge_ySn_x$ /Cu_2O is shifting towards the longer wavelength range.

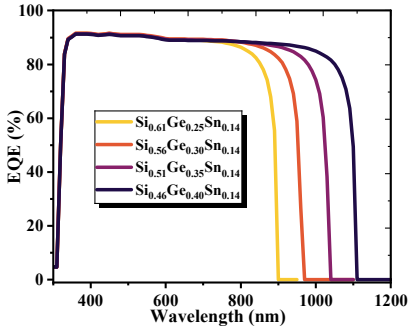

Fig.3. EQE characteristics for proposed device structure FTO/WS_2/$Si_{1-x-y}Ge_ySn_x$ /Cu_2O.

The device, which is absorbing a broad spectrum of wavelengths, is FTO/WS_2/$Si_{0.46}Ge_{0.40}Sn_{0.14}$ /Cu_2O. This shift is due to the bandgap narrowing effect due to compositional tuning.

Furthermore, Figure 4 shows the effect of varying Ge composition (0.25, 0.30, 0.35,0.40) in alloy $Si_{1-x-y}Ge_ySn_x$ with fixed Sn content of 14%, which is incorporated as an absorber layer in the PV device. This plot provides a cumulative measure of the photocurrent generation capability across the solar spectrum, which is critical for evaluating the photo-response efficiency of absorber materials.

Fig.4. Integrated short-circuit current-density curve for proposed device structure FTO/WS_2/$Si_{1-x-y}Ge_ySn_x$ /Cu_2O.

All compositions exhibit a similar trend in the initial rise of the integrated current density curve. The integrated J_{SC} continues to rise for devices having an absorber layer $Si_{0.46}Ge_{0.40}Sn_{0.14}$, while compositions with lower Ge content $Si_{0.61}Ge_{0.25}Sn_{0.14}$, plateau earlier, indicating reduced absorption in the near-infrared (NIR) range.

Table II. PV performance of proposed device structure FTO/WS_2/$Si_{1-x-y}Ge_ySn_x$ /Cu_2O

Composition of Ge	V_{OC} (V)	J_{SC} (mA-cm^{-2})	FF (%)	PCE(%)
25	0.97	28.93	86.95	24.45
30	0.88	31.43	85.99	23.91
35	0.79	34.28	84.89	23.19
40	0.72	38.09	83.72	22.97

IV. CONCLUSION

This work presents the systematically investigated the optoelectronic performance of Group IV $Si_{1-x-y}Ge_ySn_x$ ternary alloys with fixed Sn content (14%) and varying Ge composition, focusing on their applicability as absorber layers in photovoltaic devices. Through a comprehensive analysis of EQE spectra, J–V characteristics, and integrated short-circuit current density, we demonstrated that compositional tuning plays a critical role in optimizing device performance.

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