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Optical constants of silicon germanium films grown on silicon substrates

Dun Li [a,*], Xin Zhao [a], Andrew Gerger [b], Robert Opila [c], Li Wang [a], Brianna Conrad [a], Anastasia H. Soeriyadi [a], Martin Diaz [a], Anthony Lochtefeld [b], Allen Barnett [a], Ivan Perez-Wurfl [a]

[a] School of Photovoltaic and Renewable Energy Engineering, The University of New South Wales, Sydney, New South Wales 2052, Australia
[b] AmberWave Inc., Salem, New Hampshire 03079, USA
[c] Department of Materials Science, University of Delaware, Newark, Delaware 19716, USA

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ABSTRACT

Silicon germanium ($Si_{1-x}Ge_x$) is a material with high mobility and relatively low bandgap making it an attractive candidate for the bottom subcell in a multi-junction solar cell. Optical constants of $Si_{1-x}Ge_x$ films grown on silicon substrates with germanium (Ge) compositions of 77%, 82%, 85% and 88% from wavelength of 400 nm to 1450 nm at room temperature are reported. Spectroscopic ellipsometry is used to obtain the real part of refractive index for the whole wavelength range and the extinction coefficients for short wavelengths. Optical transmittance ratio of two structures being different only in the thicknesses of the $Si_{1-x}Ge_x$ films is used to extract the extinction coefficients for long wavelengths. We demonstrate that the optical constants of $Si_{1-x}Ge_x$ films grown on silicon substrates with the aid of graded buffer layers are similar to that of their corresponding bulk materials. However, the absorption coefficients of $Si_{1-x}Ge_x$ with 88% Ge determined by us at around 1000 nm is three times higher than previously interpolated results. The main reason for this discrepancy may be due to the inaccuracy of interpolation in the wavelength range where the material's bandgap changes very quickly. In addition, it should be noted that the Ge composition of the $Si_{1-x}Ge_x$ films we are able to obtain are determined to be ±1% which is much more accurate than the previous experimentally determined results which have an accuracy of ±5%.

1. Introduction

$Si_{1-x}Ge_x$ is a material with high mobility and relatively low bandgap making it an attractive candidate for the bottom subcell in a multi-junction solar cell system [1–4]. It has been reported that a III–V/SiGe dual junction solar cell grown on silicon substrate has the potential to achieve an efficiency higher than 30% [5,6]. An 18.9% efficient solar cell with this structure has been reported [7–9]. A $Si_{1-x}Ge_x$ solar cell grown on silicon substrate with the aid of a graded buffer layer has also been fabricated and optimized [10]. The germanium (Ge) composition is a critical value when $Si_{1-x}Ge_x$ is used as an active layer in a solar cell. This is because the open circuit voltage and short circuit current depend on the material's bandgap. Only 4% change in the Ge composition may lead to a change of 40 mV in the open circuit voltage [11]. The $Si_{1-x}Ge_x$ alloys in the range of $80\% < x < 90\%$ are important in the optimization of III–V/SiGe tandem solar cell as there is always a tradeoff between open circuit voltage and short circuit current depending on the composition [5]. In order to optimize the performance of III–V/SiGe tandem solar cells it is necessary to accurately know the optical constants of $Si_{1-x}Ge_x$ with small compositional changes within this range.

Despite the importance of $Si_{1-x}Ge_x$ alloys in semiconductor devices, publications about the material's optical constants are very limited. Braunstein et al. [1] provide the only available experimental determined absorption coefficient of bulk $Si_{1-x}Ge_x$ with 64%, 87.2%, 91.5% and 95.2% Ge compositions in the near-infrared range by measuring the transmittances of wafers with different thicknesses. However, the samples they used were determined to ±5% of the Ge composition. Humlíček et al. [12,13] provide refractive index of bulk $Si_{1-x}Ge_x$ with 63.5%, 75%, 83.1% and 91.4% Ge compositions with spectroscopic ellipsometry measurement. The relatively large compositional range and low composition accuracy in these reports are not accurate enough for solar cell optimization. Based on their results, optical constants with 75%, 80% and 90% Ge compositions were interpolated with the Macfarlane–Roberts expression [14,15]. It

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[*] Corresponding author. Tel.: +61 4 4912 3588.
E-mail address: dun.li@student.unsw.edu.au (D. Li).

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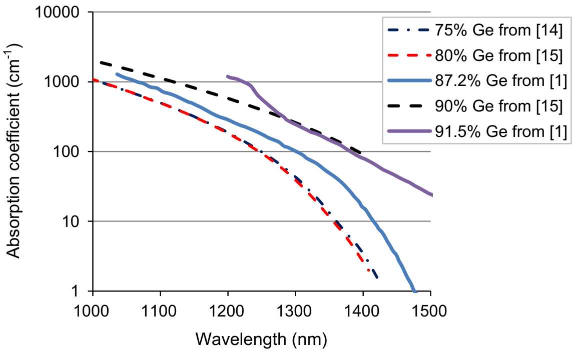

Fig. 1. Absorption coefficients of $Si_{1-x}Ge_x$ alloys with different Ge compositions from literature [1,14,15].

is worth noting that the bandgap of $Si_{1-x}Ge_x$ changes very quickly in the range of $80\% < x < 90\%$ [1]. This may limit the accuracy of results from interpolation. Fig. 1 compares the reported absorption coefficients from above mentioned literature [1,14,15]. As we can see, the absorption coefficient for the 75% Ge from [14] and 80% Ge from [15] almost have the same value. Also notice that the 91.5% Ge from [1] has similar value as that of the 90% Ge from [15] at 1400 nm but two times higher at 1200 nm. The limited and inconsistent results in literature make it necessary for us to experimentally determine the optical constants of $Si_{1-x}Ge_x$ within the narrow compositional range of interest for photovoltaic devices.

A graded buffer layer is needed to grow low threading dislocation $Si_{1-x}Ge_x$ on silicon substrates because of the lattice mismatch between silicon and $Si_{1-x}Ge_x$ [16]. In the graded buffer layer the material gradually transitions from silicon to $Si_{1-x}Ge_x$. The existence of the graded buffer layer and the thin film thickness may make the optical properties of $Si_{1-x}Ge_x$ films grown on silicon substrates different from that of bulk $Si_{1-x}Ge_x$. To the authors' knowledge, there are no previous reports on the optical constants of $Si_{1-x}Ge_x$ films grown on silicon substrates.

In this work, optical constants of $Si_{1-x}Ge_x$ films grown on silicon substrates with Ge compositions of 77%, 82%, 85% and 88% for the wavelength range of 400–1450 nm are determined. Spectroscopic ellipsometry is used to obtain the real part of refractive index for the whole wavelength range and the extinction coefficients for short wavelengths. Optical transmittance ratio of two structures being different only in the thicknesses of the $Si_{1-x}Ge_x$ films is used to extract the extinction coefficients for long wavelengths. This method takes advantage of the thick graded buffer layer which acts almost as an ideal anti-reflection coating. The Ge compositions of the $Si_{1-x}Ge_x$ films are determined to be $\pm 1\%$ with the help of high resolution X-ray diffraction scan (XRD). Our theoretical analysis of the technique employed shows the high accuracy of this approach.

2. Approach

2.1. Refractive index and short wavelength extinction coefficient

Spectroscopic ellipsometry is routinely used to determine the optical constants of thin films [17,18]. This method is based on the change in polarization state of light reflected from the surface of a sample. The measurement is recorded as two values related to the Fresnel reflectance ratio of p- and s-polarized light given by

$$\rho = \tan(\psi)e^{i\Delta} = \frac{R_p}{R_s} \tag{1}$$

where $\tan(\Psi)$ is the amplitude ratio, and Δ is the phase difference.

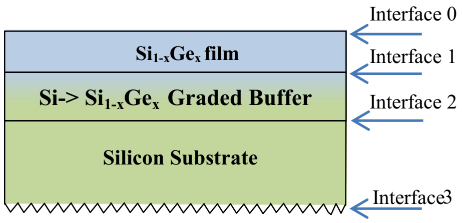

Fig. 2. Basic structure of a $Si_{1-x}Ge_x$ film grown on silicon substrate with the aid of a graded buffer layer. Due to the rough back surface the reflection from interface 3 cannot be collected by ellipsometer. There is no reflection at interfaces 1 and 2 since the gradually changed buffer layer acts almost as an ideal anti-reflection coating.

For a single layer film on a known substrate, the unknown parameters are the real part of the refractive index (n), extinction coefficient (k) and film thickness (d). Spectroscopic ellipsometry measurement can only provide two data values (Ψ, Δ) which are not adequate to uniquely determine refractive index and extinction coefficient if the thickness is not known. However, if the thickness of the thin film is known, the problem is solvable. By roughening the back surface of the sample as shown in Fig. 2, reflections from the back surface will not be collected by the detector because of its very small acceptance angle. In addition, there is no reflection at interface 1 and interface 2 as shown in Fig. 2. This is because a graded buffer layer is grown between Si and $Si_{1-x}Ge_x$ in order to grow low dislocation $Si_{1-x}Ge_x$ due to the lattice mismatch. In the graded buffer layer the materials gradually transitions from silicon to $Si_{1-x}Ge_x$. Since the Ge composition changes continually and smoothly, there is actually no clear interface at interface 1 and interface 2. The gradually varying refractive index in the thick graded buffer layer makes it act almost as an ideal anti-refection coating. In this case, all the light collected by the ellipsometer is from the reflection at interface 0 shown in Fig. 2. Therefore, the substrate can be seen as 'semi-infinite'. The film thickness and the effect of the graded buffer layer are no longer a consideration [17] and the equations for the system is fully determined.

However, it is worth noting that, when the extinction coefficient (k) is significantly smaller than the refractive index (n), it is difficult to determine each one uniquely using spectroscopic ellipsometry. The extinction coefficient can only be reliably determined with this technique when it is of the same order of magnitude as the refractive index. With this in mind, we can conclude that the extinction coefficient of $Si_{1-x}Ge_x$ films grown on silicon substrates can be uniquely determined by epectroscopic ellipsometry for a sample with rough back surface only in the short wavelength range when the extinction coefficient is large.

2.2. Long wavelength extinction coefficient

When the extinction coefficient is significantly smaller than the refractive index, the transmittance ratio of two structures being different only in the thickness of the $Si_{1-x}Ge_x$ film can be used to determine the extinction coefficient. Fig. 3 shows the transmittance of a $Si_{1-x}Ge_x$ film grown on a silicon substrate with a graded buffer layer. Because of the relatively wide bandwidth of the light probe used and the thick substrate, coherence is lost between beams that have undergone different number of reflections within the substrate. It is then sufficient to consider the intensity of the reflected wave only and disregard the phase. I_0 is the intensity of the incident light. T is the total amount of light transmitted which is given by an infinite sum of all the transmitted rays considering all possible internal reflections. R_f and R_b are the reflectivity of the front and back surfaces. R_{fi} is the internal reflectivity of the front