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Heterostructures Ge_xSi_{1-x}/Si as a material for solar cells

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In Ge-Si heterostructure system, strain and compositional changes can be used to change the fundamental indirect absorption edge. It is well known that increase in Ge content in the Ge_xSi_{1-x} shifts fundamental band edge to the longer wavelengths and causes strong increase in absorption coefficient. Theoretical description of increase in efficiency of solar cells based on this system in comparison with the silicon solar cells is given. A construction of photodiodes using heterostructure $Ge_{0.2}Si_{0.8}$/Si is proposed.

Keywords: Ge_xSi_{1-x}/Si, heterostructure, modelling.

1. Introduction

Renewed and fast growing interest of SiGe alloys began in the 80's. Searching ways towards higher PV conversion efficiencies, the multiply band gap concepts have received increased theoretical attention in the last few years. Many of dual band gap systems are based on the semiconductor couple Ge_xSi_{1-x}/Si. This is not the optimum theoretical couple for maximum system efficiency because of economic and technological criteria. The Si cell may work at a moderate concentration of infrared light non converted by GaAs (energy lower than about 1.5 eV). By changing the basic solar cell material from Si to some Ge_xSi_{1-x} alloy without much altering, if possible, solar technology can take full profit to actual know-how and future improvements [1–3].

The purpose of this work is to explore the possibilities of heterostructure Ge_xSi_{1-x}/Si materials to present by modelling how to construct Si-like solar cells showing enhanced infrared efficiencies.

Band-gap energy of Ge_xSi_{1-x} was calculated for 300 K and then experimentally checked. Absorption coefficient of Ge_xSi_{1-x} for infrared photon energies ($h\nu < 1.5$ eV) has been done and it is $\alpha = 10^1$–10^2 cm^{-1} for 1.1 eV photon energy. Enrich Ge in Ge_xSi_{1-x} coming to decrease energy gap from 1.12 eV for pure Si to 0.66 eV for pure Ge through strongly decrease in E_g curve for Ge component x = 0.85.

The crystalline, unstrained Ge_xSi_{1-x} alloys have been shown to be powerful material candidates for infrared photovoltaic conversion and Ge_xSi_{1-x} solar cells used instead of Si cells in GaAs/Si systems should improve their efficiency by up to 2 points from PV-Eye 29% to 31% for x = 0.5, up to 30% for x = 0.15 [2].

2. Simulation of solar cells efficiency

Let us analyse theoretically efficiency of barrier photocells [5,6]

$$\eta_m = \frac{kT}{E_g}(1-R)\beta f(z)\psi(x_1), \tag{1}$$

where R is the reflectivity coefficient, $\beta = (1 + sd/D_p)^{-1}$ is the surface recombination coefficient, d is the distance from fluxing surface, D_p is the holes diffusion coefficient, s is the surface recombination velocity, and

$$f(z) = \frac{y_m^2}{z(1+z-y_m)}. \tag{2}$$

In the last equation y_m is the root of equation, which is the condition for the power maximum in outside circle

$$y_m = (1+z-y_m)\,ln(1+z-y_m),$$
$$0 \le y_m \le z, \quad z = \frac{i_I}{i_s}, \quad y = \frac{i}{i_s}.$$

i_I is the fluxing current component, i_s is the diode saturation current, i is the whole current of photovoltaic cell, and

$$\psi(x_1) = x_1 \int_{x_1}^{\infty} \frac{x^2 dx}{e^x - 1} \left\{ \int_0^{\infty} \frac{x^3 dx}{e^x - 1} \right\}^{-1}, \tag{3}$$
$$x_1 = \frac{E_g}{kT_1}, \quad x = \frac{\hbar\omega}{kT_1},$$

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$\psi(x_1)$ is the function describing proportion between generation of carriers and power of electromagnetic irradiation.

Because solar irradiation is close to blackbody full irradiation, the Planck formula for $T = T_1 = 6000$ K (temperature of solar surface) was used. The diagram of f(z) is presented in Fig. 1 and the function $\psi(x_1)$ is shown in Fig. 2.

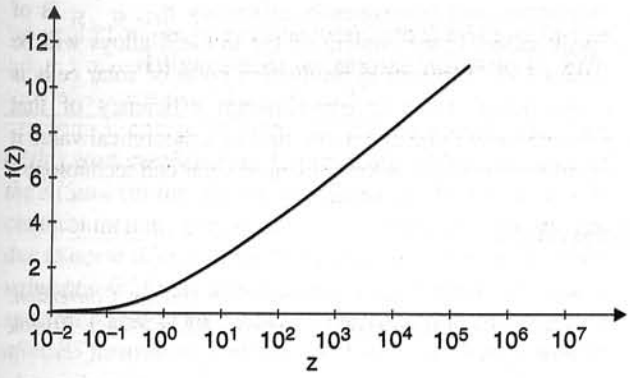

Fig. 1. Diagram of f(z) function.

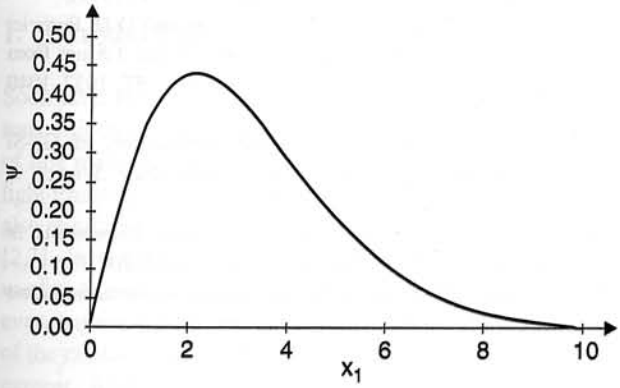

Fig. 2. Diagram of $\psi(x_1)$ function.

Analysing Eq. (1), Figs. 1 and 2 we can observe that barrier photocell can give extremely 44 points efficiency when all external and internal energy losses can be neglected. The function $\psi(x_1)$ has its maximum for about $E_g = x_1 kT_1 = 1.1$ eV, i.e., for Si band gap.

3. Theoretical considerations on heterojunction efficiency

If we could compose heterojunction with the Si and Si-like band gap material were able to increase theoretically efficiency of system over the 44% [5,6].

In Fig. 3, energetic model of photoelectrical cell with Ge_xSi_{1-x}/Si heterojunction is presented. Semiconductor of n-type (Si) with the energy gap E_g(Si) is the reflected side of heterojunction, p-type (Ge_xSi_{1-x}) with the energy gap $E_g(Ge_xSi_{1x}) < E_g$(Si) is the back side. All photons with the energy $\hbar\omega < E_g$(Si) are absorbed very weekly in n-area, and barrier arising for holes is counteracting to their flow into the irradiated surface. Photons with the energy

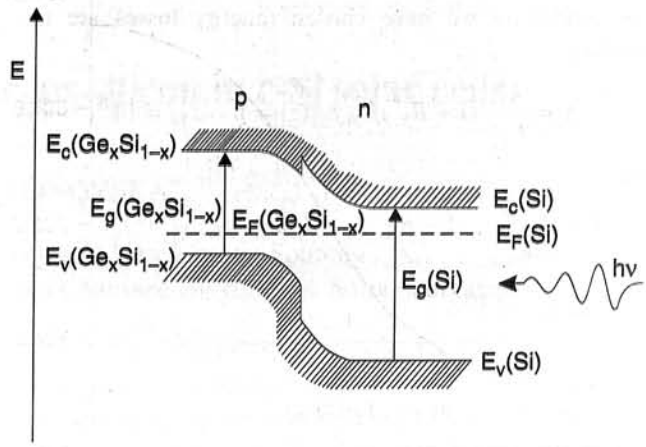

Fig. 3. Schema of energetic model of photoelectrical cell with Ge_xSi_{1-x}/Si heterojunction.

$\hbar\omega > E_g$(Si) are strongly absorbed in n-area and p-n junction is not accessible for them. Photons with the energy $\hbar\omega < E_g(Ge_xSi_{1-x})$ do not generate electron-hole couples in a junction region. That photocells are sensitive only for the range of photons energy E_g(Si) – $E_g(Ge_xSi_{1-x})$. Every Si-like material, for which E_g is less then 1.1 eV, can be chosen as a solar cell material on the base of heterojunction. However, the point is to choose material with optimal optical and electrical parameters. As we can see Ge_xSi_{1-x} is a good candidate.

Now let us consider $\psi(x_1)$ for Ge_xSi_{1-x} as a germanium component function (Fig. 4). As we notice, with Ge increasing in Ge_xSi_{1-x} alloy, the function $\Psi(x_1)$ decreases. Efficiency for system GeSi/Si is given by equation

$$\eta_{Ge_xSi_{1-x}/Si} = \eta_{Si} + \eta_{Ge_xSi_{1-x}} = A\psi(x_1)_{Si} + B\psi(x_1)_{Ge_xSi_{1-x}}. \quad (4)$$

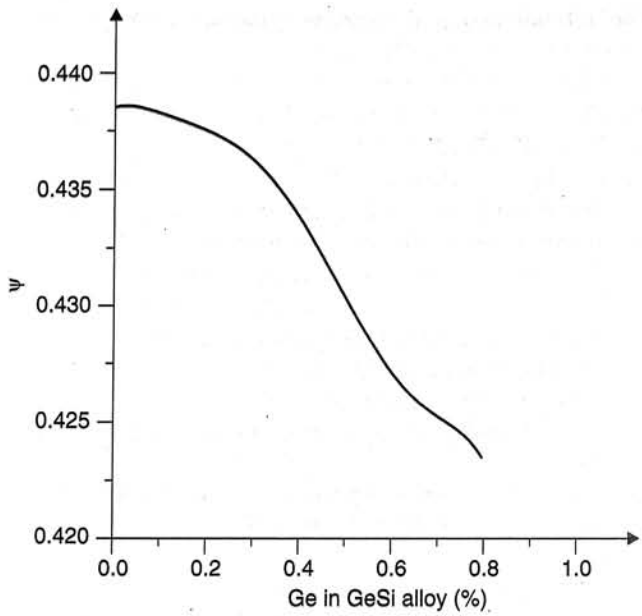

Fig. 4. $\psi(x_1)_{Ge_xSi_{1-x}}$ function for x Ge composition, $0 < x < 0.8$.

For modelling we have chosen (energy losses are neglected)

$$A = \frac{kT}{E_{g_{Si}}}(1 - R_{Si})\beta_{Si} f_{Si}(z) = 1, \quad z_{Si} = 10^4, \qquad (5)$$

and

$$B = \frac{kT}{E_{g_{Ge_xSi_{1-x}}}}(1 - R_{Ge_xSi_{1-x}})\beta_{Ge_xSi_{1-x}} f_{Ge_xSi_{1-x}}(z) = \frac{1}{p},$$

$$z_{Ge_xSi_{1-x}} = 10^2$$

$$\frac{1}{p} = \frac{f_{Ge_xSi_{1-x}}(z)}{f_{Si}(z)} = 0.39. \qquad (6)$$

The results of that simulation of $\eta_{Ge_xSi_{1-x}/Si}$ [see Eq. (2)] for $0 < x < 0.8$ are presented in Fig. 5.

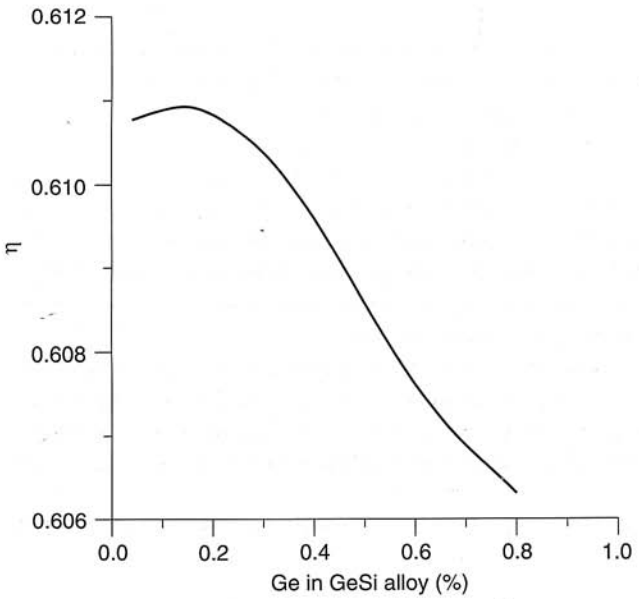

Fig. 5. Efficiency $\eta_{Ge_xSi_{1-x}/Si}$ versus x composition, $0 < x < 0.8$.

4. Conclusions

Ge_xSi_{1-x} layers enriched with Ge increase absorption coefficient in a fundamental band, i.e., from $\alpha = 10^2$ cm^{-1} to $\alpha = 10^3$ cm^{-1}. It is additional advantage allowing for efficiency increase.

For Ge composition x = 0.1–0.2 the $\psi(x_1)$ function has its maximum and consequently efficiency $\eta_{Ge_xSi_{1-x}/Si}$ is of the peak value. If the content of Ge in GeSi alloys will be less then 15%, increase in production costs of solar cells is not significant. Even if experimental efficiency of that heterojunction will be about one-half of a theoretical value it is satisfying for future development of solar cell technology.

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