

Modelling and analysis of temperature-dependent carrier lifetime and surface recombination velocity of Si–ZnO heterojunction thin film solar cell

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ZnO–silicon heterojunction solar cell having high efficiency and high fill factor is structured and simulated to study its photovoltaic properties under different device temperature. Current–voltage measurement of dimensionally optimised device structure revealed up to 20.44% efficiency and 83.66% fill factor at $1 \Omega\text{-cm}^2$ external series resistance at 300 K. Measured current–voltage shows decrease of open-circuit voltage from 659.13 to 109.1 mV and short-circuit current from 40.65 to 39.5 mA/cm² with increase of device temperature. Quasi-steady-state photoconductance measurement reveals small recombination current and long Shockley Read Hall lifetime under the selected temperature range indicating superior performance of the device. Adverse effect of surface recombination velocity at rear surface of the device is observed at lower temperature (100–600 K) range indicating better majority carrier collection at very high temperature 700 K and above.

1. Introduction: Heterojunction solar cell (SC) fabricated by deposition of transparent conducting zinc oxide (ZnO) on a single crystalline silicon (c-Si) is a burning topic of present days in photovoltaic industry, because of low-temperature handling and cheapness [1–3]. In this regard, superior blue response is a prominent characteristic of heterojunction ZnO–Si SC. In addition, low sheet resistance and prodigious transparency of ZnO thin film due to large bandgap (3.3 eV) are applicable qualities for optoelectronics devices. Moreover, double-band photon absorption that is high energy ultra-violet photons absorbed in ZnO layer and low energy visible range photons absorbed in c-Si, improves the quantum efficiency (QE) but not up to the desired level in such devices. Those devices are fabricated by different methods such as spray pyrolysis, thermal evaporation, molecular beam epitaxial, sol–gel method and laser deposition [4]. In addition, some researchers showed improvement of thin ZnO film quality and hence overall performance of SC based on it at high temperature [2, 5]. In some other works in the art, temperature-dependent diode parameters and current density–voltage (J–V) plot were investigated [6, 7]. Such research directions lead us to study temperature dependency of minority carrier lifetime and other prominent parameters like surface recombination velocity (SRV, S_r) in ZnO/Si-based SC.

The presented work is a simulation study of slightly modified existing ZnO/Si SC and its characterisation based on distinguished parameters under different device temperature. In order to improve efficiency, the Si back surface field (BSF) in the existing device is replaced with hydrogenated microcrystalline silicon oxide ($\mu\text{c-Si}_{1-x}\text{O}_x\text{:H}$) as in the proposed one. The proposed device structure is then calibrated with experimental results of the existing work (having Si BSF) in the literature. Temperature dependency of major SC parameters such as minority carrier lifetime, SRV, open-circuit voltage (V_{OC}) and short-circuit current (J_{SC}) of the presented structure is thoroughly investigated throughout the task. AFORS-HET (Ver. 2.5) is used for all numerical simulation purposes in the work.

2. Proposed SC structure: Novel heterojunction SC consisting Al/a-ZnO(n)/c-Si(Interface)/c-Si(p)/c-Si(Interface)/ $\mu\text{c-Si}_{1-x}\text{O}_x\text{:H}(p+)$ /Al structure shown in Fig. 1a is designed in the simulator. The emitter layer in the proposed structure consists of highly boron (B) doped n-type amorphous ZnO (a-ZnO). In the work the boron

doping is used for better ohmic contact at the front transparent conducting oxide at the small expense of its transparency. Electrical and optical parameters of c-Si base layer needed in the simulation is adopted from [9] in the presented work. Hydrogenated microcrystalline oxide of silicon BSF carrier reflector is used for better collection of hole at back contact [10]. Molar fraction of the oxygen in the BSF layer is taken to be a reasonable value $x=0.2$. Electrical and optical modelling parameters for $\mu\text{c-Si}_{1-x}\text{O}_x\text{:H}$ and c-Si are assumed to be the same in the simulation structure. Modelling of electrical parameters like energy bandgap, electron mobility, hole mobility, effective density of states (DOS) of conduction band (CB) and that of valence band (VB) of a-ZnO are coined from similar work done by Nawaz *et al.* [11]. Other parameters such as static dielectric constant, electron affinity and electron and hole thermal velocity of a-ZnO are taken from [12]. The major design parameters of the model are displayed in Table 1. Major recombination models like Shockley Read Hall (SRH), bulk band-to-band and Auger recombination are applied to a-ZnO layer. In addition, DOS of different active layers are modelled simply by band tails states of CB and that of VB in association with bandgap impurity having Gaussian distribution of donor/acceptor type. DOS modelling for $\mu\text{c-Si}_{1-x}\text{O}_x\text{:H}$ is based on the report presented in [13], whereas for c-Si inbuilt DOS modelling in the simulator is used. On the other side, the DOS modelling of a-ZnO is based on the similar work presented in [14].

Effect of temperature on energy bandgap and on mobility of the presented SC layers is negligible, except for main absorber layer base c-Si, because, the main contribution of carrier collection is provided by this layer only. Passler model for temperature dependent energy bandgap, given by the following expression, is applied for the base c-Si layer in the simulation because of its superiority then other similar models, as stated in the literature

$$E_g(T) = E_g(0) - \alpha \Theta \left[\gamma + \frac{3\Delta^2}{2} \left(1 + \frac{\pi^2}{3(1+\Delta^2)} \right) \chi^2 + \frac{3\Delta^2 - 1}{4} \chi^3 + \frac{8}{3} \chi^4 + \chi^6 \right]^{1/6} - 1 \quad (1)$$

The model parameters used are taken from [15] which are given as: energy bandgap at temperature $T=0$ K is $E_g(0) = 1.17$ eV,

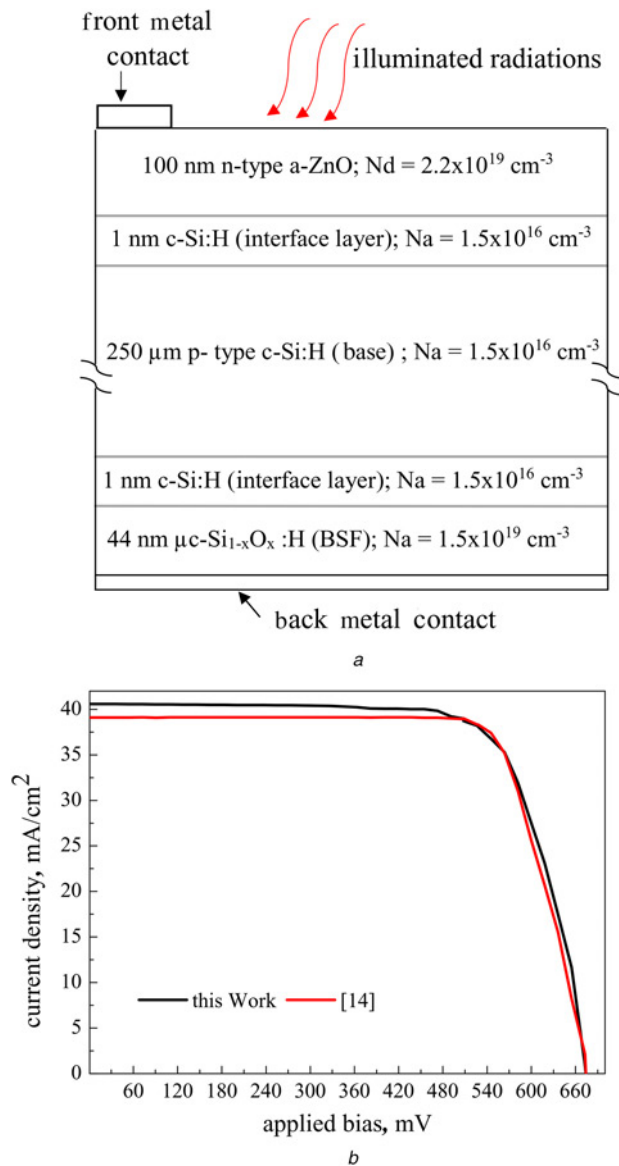


Fig. 1 Proposed solar cell device schematics with characterisation
a Schematic representation of the proposed ZnO/Si heterojunction SC layers where doping profile of each layer is assumed to be uniform and $N_d = 2.2 \times 10^{19} \text{ cm}^{-3}$ and $N_a = 1.5 \times 10^{19} \text{ cm}^{-3}$ represent optimum donor and acceptor doping concentrations of n-type and p-type layers, respectively
b Current–voltage plot of the proposed model and experimental report in [8] at $N_d = 1 \times 10^{16} \text{ cm}^{-3}$ at 300 K, under the illumination of AM 1.5, validating the simulated proposed model

$\alpha = 3.23 \times 10^{-4} \text{ eVK}^{-1}$, $\Theta = 446 \text{ K}$, $\Delta = 0.51$, $\chi = (2T/\Theta)$ and $\gamma = ((1 - 3\Delta^2)/(\exp(\Theta/T) - 1))$.

The mobility model used in the simulation is based on phonon scattering mobility (μ_L) only, as given below. The reason is its dominance upon other scattering effects in moderately doped c-Si

$$\mu_L = \mu_{L0} \left(\frac{T}{300} \right)^{-\ell + (cT/300)} \quad (2)$$

where mobility at room temperature are 1041 and $412.9 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ for electron and hole, respectively (as inbuilt in the simulator). The correction factors, ℓ and c are 2.45 and 0.07 for electron and 2.16 and 0 for hole, respectively [16].

3. Theoretical validation with experimental result: The validity of the proposed structure is done by comparing its J–V characteristics with that of experimental based result of similar device as presented in [8]. The SC evaluating parameters are showing super correlation at 300 K in both the devices and are highlighted in Table 2. The presented model is well calibrated with similar experimental work proposed in the literature as evident from Fig. 1*b* as well. However, in case of simulation slightly greater values of these parameters is observed as compared to the reference. This is due to the use of new material as BSF layer in the presented one.

In order to model optically fit ZnO layer involved, the refractive index data used in the simulation is deduced by fitting it with experimentally obtained data [17]. Refractive index of ZnO used is shown in Fig. 2 illustrating that both the propagation (n) and the extinction (k) coefficients of simulated (inbuilt in AFORSE-HET) and practical methodologies are similar in the wavelength range of interest (300–750 nm). The divergence in the n data between the two methodologies beyond 750 nm may be due to densely packed nanopillars structures used in the experimental case, whereas flat thin film is considered in the simulation. Values of n and k for c-Si and $\mu\text{c-Si}_{1-x}\text{O}_x\text{:H}$ are assumed to be the same and are adopted from the inbuilt data in the simulator.

4. Result and analysis: A symmetric structure Al/a-ZnO/interface/c-Si base/interface/a-ZnO/Al is modelled to measure effective minority carrier lifetime using quasi-steady-state photoconductance (QSSPC) method. In the method a slowly varying light pulse is exposed to the sample (symmetric structured) and conductivity (σ_{sem}) is measured. In addition, photocurrent (J_{pho}) of a SC fabricated using the same sample is measured. The effective lifetime (τ_{eff}) of carriers is then calculated as follows [18]:

$$\tau_{\text{eff}} = \frac{\sigma_{\text{sem}}}{J_{\text{pho}}(\mu_n + \mu_p)} = \frac{\Delta n}{(d\Delta n/dt)} \quad (3)$$

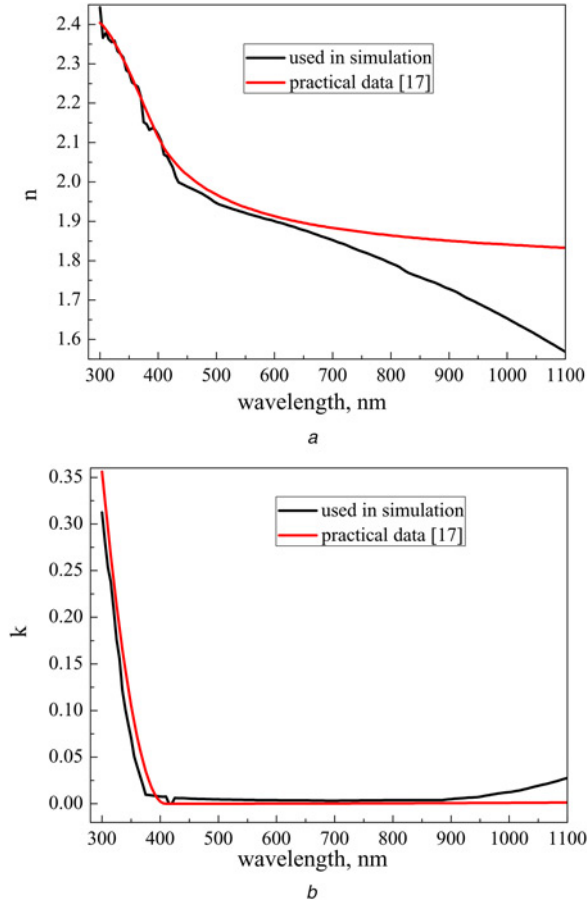
where μ_n and μ_p are electron and hole mobility, respectively.

Table 1 Electrical and optical parameters of the materials used

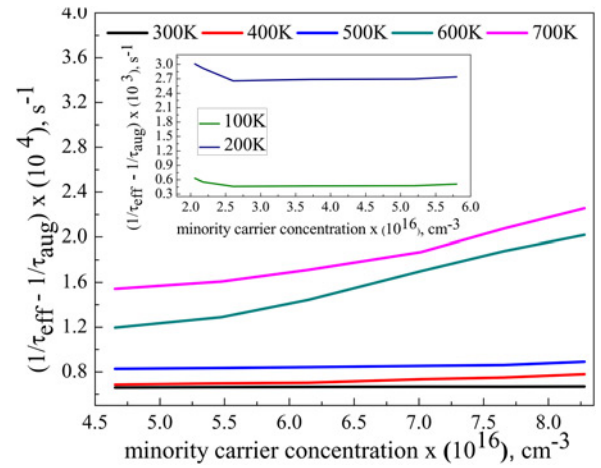
Parameters		a-ZnO	c-Si	$\mu\text{c-Si}_{1-x}\text{O}_x\text{:H}$
mobility	electron	100	1041	1
	hole	10	412.9	1
Auger coefficient	electron	1.12×10^{-31}	9.9×10^{-32}	0
	hole	1.12×10^{-31}	2.8×10^{-31}	0
band-to-band recombination coefficient		1.2×10^{-12}	9.5×10^{-15}	9.5×10^{-15}
effective DOS of	CB	2.2×10^{18}	2.84×10^{19}	2.0×10^{19}
	VB	1.8×10^{19}	2.68×10^{19}	2.0×10^{19}
bandgap at 300 K		3.3	1.124	1.124
thermal velocity	electron	3×10^5	1.0×10^7	1.0×10^7
	hole	1.5×10^5	1.0×10^7	1.0×10^7
dielectric constant		8.12	11.9	11.9
electron affinity		4.3	4.05	4.05

Table 2 J–V measurement

Parameters	V_{OC} , mV	J_{SC} , mA/cm ²	Efficiency, %	Fill factor, %
this work	654.5	40.60	20.44	83.66
ref. [8]	622.1	37.7	19.0	81.0

**Fig. 2** Simulated and experimental refractive index validation for ZnO layer
a Refractive index (n) of ZnO
b Extinction coefficient (k) of ZnO

AFORSE-HET simulation of the symmetrical structure is used for the record of excess minority carrier concentration, Δn and the carrier generation, $G(=d\Delta n/dt)$. The light exposed to the symmetrical device is a standard AM 1.5 illuminations (average incident irradiation of the sun in middle Europe in summer at noon) inbuilt in the AFORSE-HET simulator. The photon flux exposed to the device is increased from one time to six times the standard photon flux provided by the simulator, in order to generate different excess minority carrier concentrations. The average excess minority carrier and generation are given as, $\Delta n_{avg} = (1/X) \int_0^X \Delta n dx$ and $G_{avg} = (1/X) \int_0^X G dx$, where X stands for the width of the base (c-Si) layer. The effective lifetime is then calculated as $\tau_{eff} = (\Delta n_{avg}/\Delta G_{avg})$. In addition, inverse Auger lifetime is obtained by a well-known equation given as [19], $(1/\tau_{Aug}) = C_a \Delta n$. The ambipolar Auger coefficient $C_a = 1.66 \times 10^{-30} \text{ cm}^6 \text{ s}^{-1}$ as reported in [20]. A plot of Auger corrected net inverse lifetime $((1/\tau_{eff}) - (1/\tau_{Aug}))$ of minority carrier is plotted against the scaled average excess minority carrier density, $((N_a + \Delta n_{avg})/qXn_i^2)$ for different device temperature ranging from 100 to 700 K is shown in Fig. 3. Effect of lower temperature such as 100 and 200 K is shown in the inset of the figure. As the temperature decreases the emitter saturation current density (J_e)

**Fig. 3** Auger corrected inverse lifetime plotted against the excess minority carrier density

decreases according to the equation below [21]:

$$J_e a T^3 \exp\left(\frac{-E_g}{k_b T}\right) \quad (4)$$

SRH lifetime of minority carrier (τ_{SRH}) in bulk of c-Si base layer and J_e are calculated based on (5). These values are listed in Table 3

$$\frac{1}{\tau_{eff}} - \frac{1}{\tau_{Aug}} = \frac{1}{\tau_{SRH}} + 2J_e \frac{(N_a + \Delta n_{avg})}{qXn_i^2} \quad (5)$$

The elementary charge and intrinsic carrier concentration of base region are denoted by q and n_i , respectively. As evident from the calculation, J_e is increasing with the rise in temperature. As a result, the open-circuit voltage decreases according to the following equation:

$$V_{OC} = \frac{kT}{q} \ln \left[\frac{J_{SC}}{2J_r} + 1 \right] \quad (6)$$

Here J_r denotes heterojunction reverse saturation current which is commensurate to J_e . As temperature (T) increases, V_{OC} increases linearly but it decreases with rise in J_r . However, decreasing of V_{OC} with temperature as shown in Fig. 4 evidences the dominance of J_r over direct T dependency. Enlargement of J_r along with temperature manifests boosting of electron–hole recombination at the edge of the depletion region which is also observed in the work of Mackel and Varner [22]. Variation of J_{SC} and V_{OC} with change in temperature is depicted in Fig. 4. It is vivid that V_{OC} is decreasing nearly linearly with large step sizes. On the other hand, exponentially decrease of J_{SC} is observed as temperature rises. The variation of J_{SC} with temperature is studied further by QE measurements.

Table 3 Calculated values of SRH lifetime and J_e

Temperature, K	τ_{SRH} , s	J_e , A/cm ²
100	2.17×10^{-3}	1.60×10^{-16}
200	3.76×10^{-4}	3.57×10^{-16}
300	1.56×10^{-4}	2.33×10^{-15}
400	3.50×10^{-4}	2.04×10^{-14}
500	1.98×10^{-4}	2.34×10^{-14}
600	1.55×10^{-4}	5.92×10^{-14}
700	1.47×10^{-4}	8.46×10^{-14}

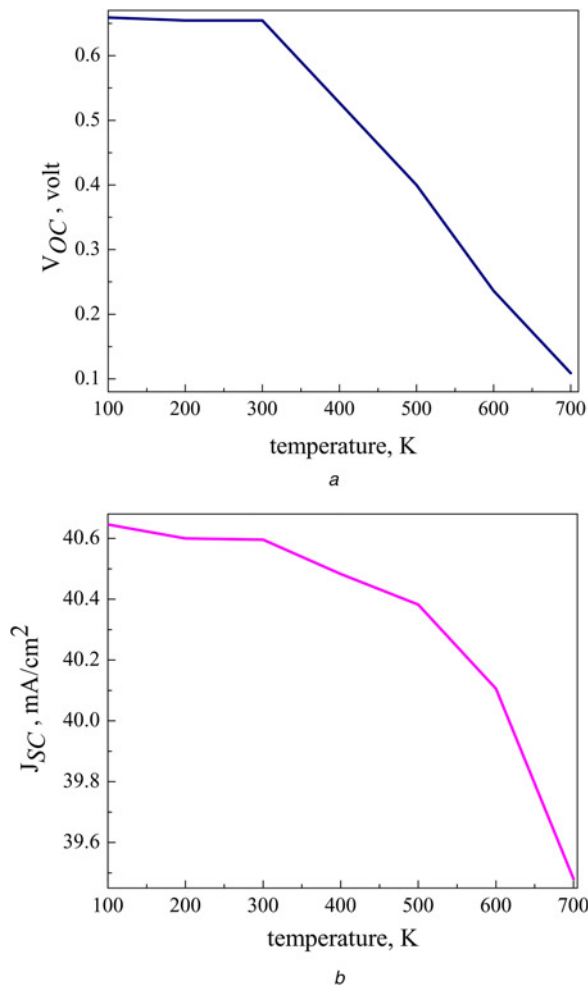


Fig. 4 Temperature effect on device performance
a Plot of V_{OC} versus temperature
b Plot of J_{SC} versus temperature

QE both external QE (EQE) and internal QE (IQE) at different device temperatures of the proposed SC model are depicted in Figs. 5a and b, respectively. A minimal point corresponding to lowest charge collection is observed at around 415 nm wavelength (at 300 K) of the illuminated light in the EQE plot. The minimal point corresponds to the illuminated photons having minimum absorbable energy which can be absorbed in ZnO emitter layer. Other lower energy photons are absorbed by the c-Si base layer. However, decreasing EQE with rise in temperature justify the charge collection efficiency of the device is also decreasing as the device temperature is increasing. Mobility of the charge carriers increases with rise in temperature according to the mobility model. On the other side, photocurrent is inversely proportional to the mobility as shown in (3) which justifies the observed characteristics of QE. Decreasing values of IQE with reference to increase in temperature as discovered in the figure confirms better photon to electron-hole pair conversion efficiency at lower temperature. In addition, minute variation in photon to charge carrier conversion is observed at lower temperature. These may be attributed to less recombination at the edge space charge region at that temperature.

SRV, S_r against excess minority carrier density for different temperature is plotted based on (7) as depicted in Fig. 6. However, variation of S_r with respect to excess minority carrier density under lower temperature is shown inside the inset of the figure

$$\frac{1}{\tau_{eff1}} - \frac{1}{\tau_{SRH}} = \frac{2S_r}{X} \quad (7)$$

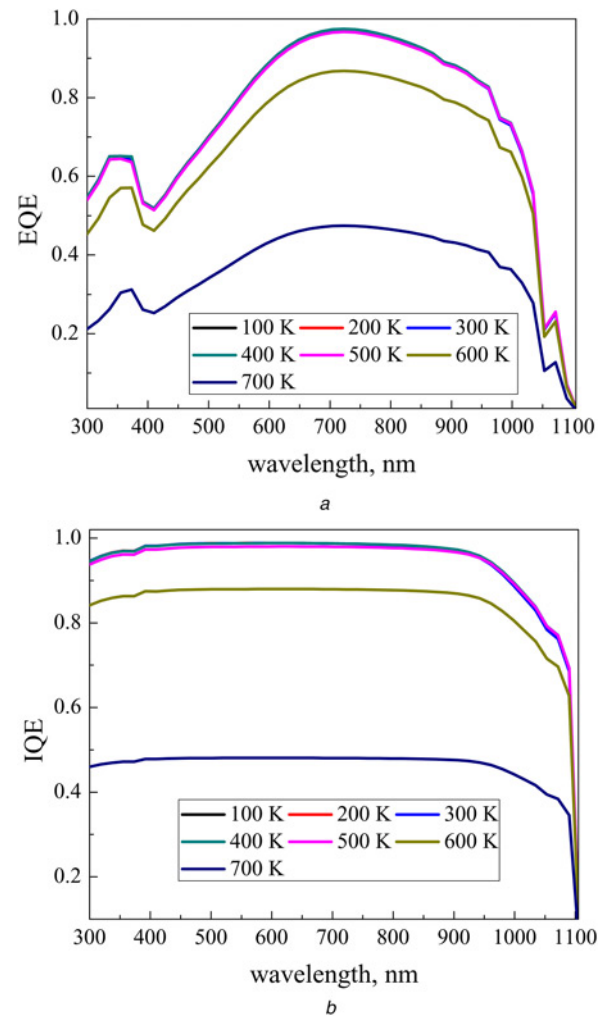


Fig. 5 QE at different temperature
a EQE
b IQE

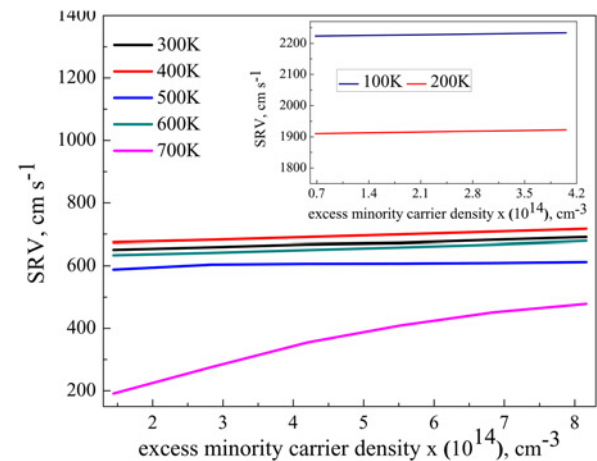


Fig. 6 Variation of SRV, S_r with minority carrier concentration under different temperature (100–700 K)

A symmetric structure $Al/\mu c - Si_{1-x}O_x:H/interface/c-Si base/interface/\mu c - Si_{1-x}O_x:H/Al$ is simulated for effective lifetime τ_{eff1} . The calculated τ_{SRH} along with X is used in (6) to calculate S_r for different temperature. Linear increase of S_r with the increasing of excess minority carrier concentration is due to the presence of more defect states at the rear surface of the device.

At the lower side of the temperature range S_r undergoes minute decrease in its value. However, at the other end of the range it becomes distinguishably smaller indicating better carrier collection there. In fact, the overall S_r is decreasing as the temperature rises under its range of interest. This is due to smaller SRH lifetime at higher temperature.

5. Conclusions: Material used in BSF layer of a novel existing single heterojunction ZnO on c-Si-based SC is replaced by $\mu\text{c} - \text{Si}_{1-x}\text{O}_x\text{:H}$ and is modelled in AFORSE-HET simulator and finally studied. The proposed simulated model provides an efficiency of 20.44% and fill factor of 83.66% is its optimum value which is a good result compared to the state-of-the-art models. QSSPC method reveals that the model provides injection-dependent effective lifetime of minority carrier and V_{oc} of the order of 10^{-4} s and 654.55 mV at 300 K, respectively. Decrease of V_{oc} with rise in temperature as observed is attributed to decrease of J_e . Due to recombination, J_{sc} decreases with rise in temperature. Finally, the study revealed that S_r is comparatively small at higher temperature and large at low temperature.

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