Effect of the lattice mismatch on the efficiency of the GaAs nanowire/Si substrate solar cell

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Abstract. The effect of the crystal lattice mismatch between single p-GaAs nanowire grown on p-Si substrate on the solar cell efficiency is studied. The study is performed by measuring the I-V curves under red (wavelength=650 nm) laser illumination. The measurement of the single nanowire was done by conductive atomic force microscopy (C-AFM). The measured curve was reproduced by numerical simulations accounting piezoresistance and piezoelectric effects. The analysis demonstrated the presence of the tensile (2%) zinc blend insert at the interface between nanowire and substrate induced by crystal lattices mismatch. Strained insert at the interface changes the polarity of the photogenerated current and increases the efficiency by 2 times.

1. Introduction
GaAs nanowires (NWs) grown on low-cost lattice-mismatched substrates provide a possibility of creating solar cells with high absorption of solar light with low consumption of GaAs material[1,2]. To increase the efficiency of the cells, additional approaches are demanded. Tandem solar cell consisting of a silicon substrate and GaAs nanowires array[3,4] is among these approaches currently being investigated.

Recently it was shown that growth of the GaAs NWs on the (111) Si substrate leads to the formation of the interface energy barrier which affects the solar cell efficiency[5]. The effect of the induced barrier in the numerical model for simplicity has been accounted by adding the fixed positive electric charge to the NW/substrate interface. However, for proper modeling piezoresistance[6] and piezoelectric[7] effects should be considered. The aim of this work was to study the effect of the lattice mismatch on the efficiency of the wurtzite GaAs NW/Si substrate solar cell.

2. Samples and methods
Wurtzite GaAs nanowires were grown in (111)B direction under 20 nm Au nanoparticles on p-Si (111) substrate. The growth was done in a molecular beam epitaxy chamber with Be p-type doping (10^{17}-10^{18} cm^{-3}). The substrate also was p-type doped with an impurity level of 10^{16} cm^{-3}. The length of nanowires was 6 µm and a diameter d=100±20 nm [8]. NWs were passivated by covering a 7-nm AlGaAs layer to reduce the density of surface non-radiative recombination centers. Conventionally, a zinc blend phase forms at the first stage during the growth of the wurtzite GaAs nanowires on the Si
substrate [9]. Thus, a zinc blende (ZB) insert with a thickness of ~10 nm was anticipated at the bottom of the NW. Details of the NW growth are presented elsewhere [5].

Measurement of the I–V curves on a single NW was performed by conductive atomic force microscopy (C-AFM) [10]. The experiment was done using NTEGRA AURA (NT-MDT, Russia) scanning probe microscope equipped with conductive HA_NC/W2C + (NT-MDT) probes. For the I–V curves measurement, the grounded probe was contacted to the NW top (see figure 1 (a)) and bias voltage was applied to the second contact created to the silicon substrate. Since the system detecting the probe position is equipped with a red laser with a wavelength of ~650 nm and a power density of 10^4 W/m^2, the NW also was illuminated by this laser during the measurement.

![Figure 1. (a) Measurement of the I-V curve of single GaAs NW by C-AFM (b) Scheme of the positioning of the parameters implemented in the model.](image)

Modeling of the I–V curves under red laser illumination was performed in 2D with cylindrical symmetry using the Atlas Silvaco software package [11]. The model replicated cylindrical GaAs with a diameter of 100 nm and a length of 6 µm placed on the Si substrate. Si substrate in the model had an affinity (conduction band minimum CBM, E_c) of 4.05 eV and a p-type doping level of 10^16 cm^-3. The NW was also p-type doped with a level of 10^17 cm^-3. The bottom contact between the Si substrate and a sample holder was set as Ohmic and the top contact with the NW was a Schottky-type with a barrier height of 0.54 eV [12]. Universal Schottky tunneling model accounting for tunneling across the Schottky barrier, recombination, and thermionic emission was used. The current was calculated accounting band-to-band and surface recombination. The mobility of holes was 0.1 cm^2/(V⋅s) [13].

Illumination by the red laser with a wavelength of ~650 nm and a power density of 10^4 W/m^2 was set with uniform space distribution and normal incident on the side surface of the NW. Lattice constants mismatch of GaAs and Si (~4%) leads to the compression of the GaAs lattice in the parallel to substrate direction at the NW/substrate interface. However, in perpendicular to the substrate direction, the NW is exposed to the tensile strain which can be estimated as 2%, according to the doubled ratio of the C_{13} and C_{33} GaAs elastic constants. Tensile strain exponentially decreased along the NWs at the length z (10-30 nm) [14]. Both piezoresistance and piezoelectric effects caused by lattice mismatch were included in the model during the calculations of I–V curves. The piezoelectric effect induces fixed charges of opposite polarities. These charges (−Q_f and Q_f) were placed at the top and bottom planes of the ZB insert with a z-thickness at the NW/substrate interface (figure 1(b)). The polarity of the charges was set according to the tensile deformation in the z-direction of the insert and the (111)B direction of the NW growth [15]. The Q_f charges per 1% strain for the ZB...
GaAs was $1 \cdot 10^{12}$ cm$^{-2}$ due to the piezoelectric constant ($e_{14} = -0.16$ C/m$^2$ [7]). The piezoresistance effect was included by changing the bandgap $E_g=1.22$ eV and the CBM $E_c=4.19$ eV of the insert under tensile strain into the model [6]. CBM of the unstrained ZB and WZ GaAs was 4.07 eV. During the modeling, the thickness $z$ of the insert was varied in the range 3-30 nm to obtain the best fit with the experiment.

3. Results and discussion

I–V curve (black solid) measured on single GaAs NW by C-AFM is presented in figure 2. The bias voltage was applied to the substrate and a negative open-circuit voltage ($V_{oc}$) is detected. I–V curve calculated by a model which does not include an effect of the crystal lattice mismatch (without strained ZB insert at the NW/substrate interface) is represented as a red dashed line in figure 2. The sign of the open-circuit voltage ($V_{oc}$) for the red curve is positive. The sign of the open-circuit voltage depends on the polarity of the photocurrent, which is controlled by the balance of the Schottky-barrier and the hetero barrier (NW/substrate). For proper modeling, a strained ZB insert was added to the model. The insert with the thickness $z=20$ nm gives good agreement between the experimental and calculated I-V curve (black dashed curve). It is worthy to note that the strained ZB insert increases the efficiency of the solar cell by ~2 times (areas under black and red curves). This is due to the low solar efficiency of the Schottky barrier which dominates in the model represented by the red curve. Strain at the NW bottom increases the hetero barrier (Si/GaAs NW) height and changes the sign of the photocurrent and the efficiency of the whole solar cell.

![Figure 2. I-V curves of the p-GaAs NW grown on p-Si substrate. Measured curve of the NW (black solid) and calculated curves with accounted tensile strain at the NW bottom induced by lattice mismatching (black dashed) and without tensile strain (red dashed curve).](image)

4. Conclusion

Thus, p-GaAs NW/p-Si substrate solar cell was studied by measuring the I–V curves under red laser illumination by C-AFM. Observed open-circuit voltage of the NW-substrate solar cell is governed by the balance of the Au cap/GaAs NW and GaAs NW/Si barriers. Sign of the photogenerated current indicates an impact of the GaAs NW/Si barrier increased by a strain which is induced due to GaAs/Si lattice mismatch. Numerical calculation accounting piezoresistance and piezoelectric effects shows a presence of the 2% tensile along NW in the 20 nm region at the NW/substrate interface. The
calculation shows ~2 times increasing of the solar cell efficiency due to the presence of the strained GaAs NW/Si substrate interface.

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