Figure-of-merit evaluation of gold-hyperdoped silicon for photovoltaic applications

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Motivation

We used terahertz spectroscopy to study charge carrier lifetime in hyperdoped silicon, and found that lifetime is highly dependent on ion-implantation energy. This study sheds light on optimization of the hyperdoping process and evaluation of promising systems for intermediate band photovoltaics.

Introduction

Intermediate band photovoltaics:

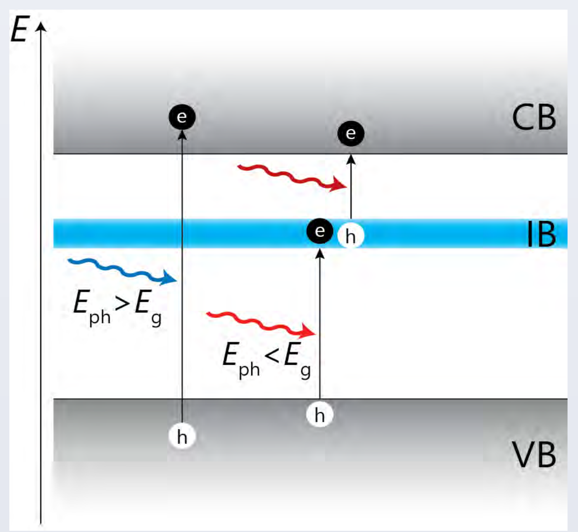

Figure 1 – Energy band diagram of an intermediate band semiconductor

Efficiency of a solar cell can be enhanced by harvesting a much larger portion of the solar spectrum. This could be achieved by introducing an intermediate band in the semiconductor band structure. Two lower energy photons are absorbed in a two-step process creating one high energy electron. Intermediate band photovoltaics has theoretical efficiencies as high as 63%. Laser hyperdoping is a viable method to introduce large concentrations of dopants and enabling intermediate band formation.

Laser hyperdoping:

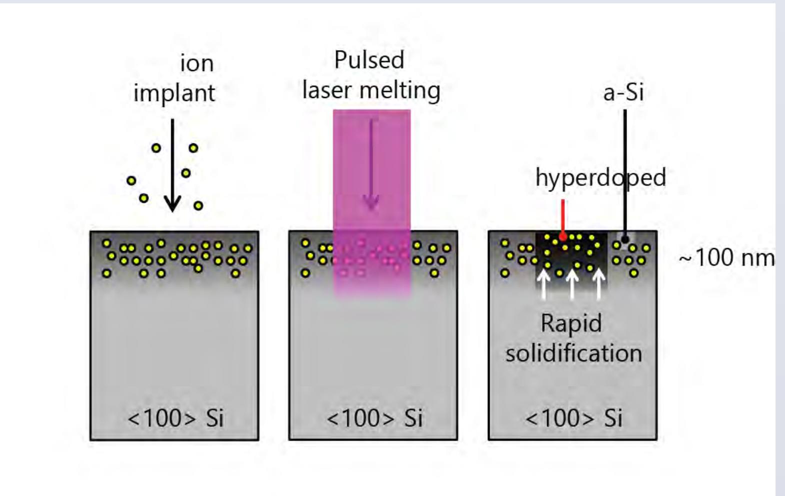

Figure 2 – Hyperdoping process. Figure adopted from Ref [1]

The process of ion implantation followed by pulse laser melting (PLM) results in deep level dopants at supersaturated concentrations in a single crystalline structure. The resulting hyperdoped Si can achieve dopant concentrations as high as 10^{20} atoms/cm^3 [1].

Figure-of-merit:

Without optimizing all parameters in a solar cell, using the figure-of merit (FOM), we evaluate the potential of any hyperdoped system. The FOM compares charge carrier transit time to the lifetime of carriers in the intermediate band layer [2]. In detail, reaching the highest FOM requires optimizing these parameters:

- Band gap – E_g
- Absorption coefficient – α
- Carrier lifetime – τ
- Mobility – μ

Figure 3 shows FOM of sulfur-hyperdoped silicon. In that study, the carrier lifetime decreases with increasing dopant concentration, leading to a small FOM at high dopant concentrations [3].

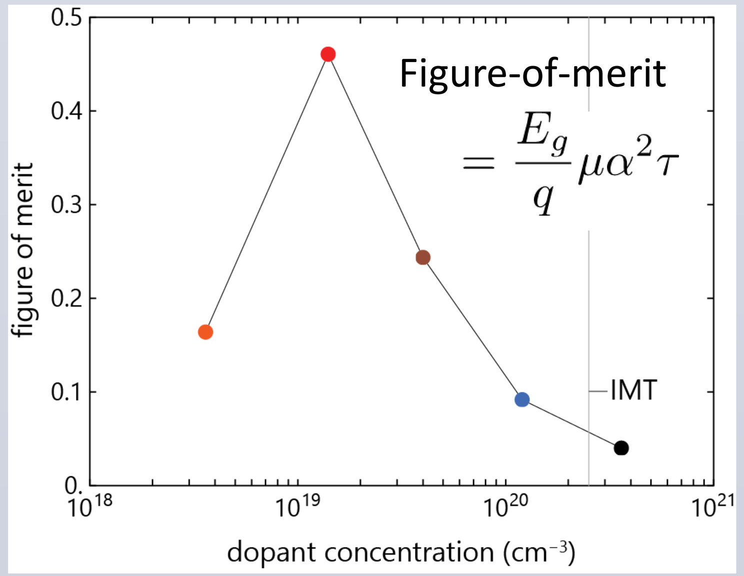

Figure 3 – Figure of merit of S-hyperdoped Si. Figure adopted from Ref [3]

Experiments

Carrier lifetime is a crucial parameter for optimizing FOM. We use terahertz spectroscopy to study carrier lifetime of gold-hyperdoped silicon (Si:Au) samples with different Au dose (1e12 to 1e15 cm^{-2}) and different ion-implantation energies (50, 110 and 300 keV).

Time resolved terahertz (THz) spectroscopy:

A non-contact photoconductivity measurement is used to determine the carrier lifetime. The carriers in the sample are excited using an optical pump pulse and then probed by a THz pulse. Conductive carriers attenuate the THz probe, and hence the THz transmission amplitude is proportional to the conductivity of the samples.

$\Delta T \propto \Delta\sigma$

ΔT – Change in THz transmission

$\Delta\sigma$ – Change in conductivity

The laser beam is split into three paths; optical excitation, THz generation and THz detection.

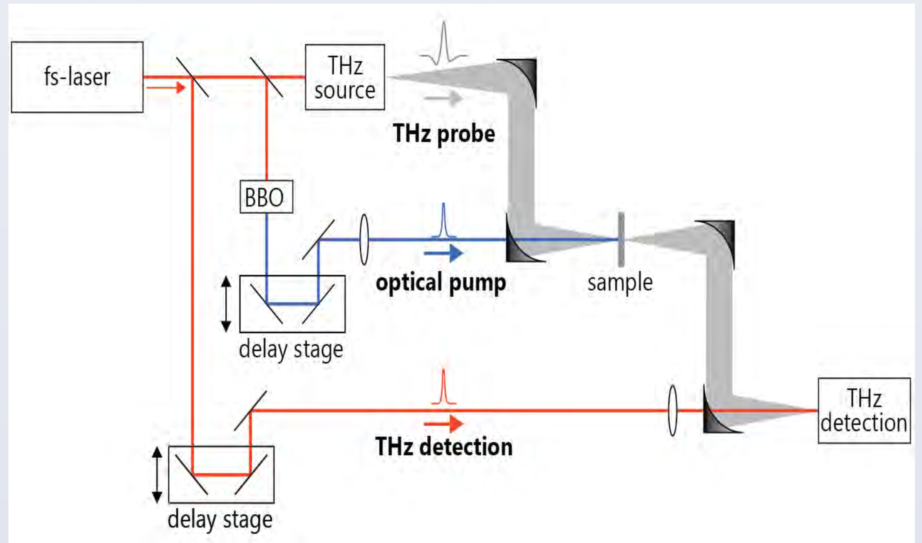

Figure 4 – Schematic diagram of the experimental setup

The time evolution of the photoconductivity is monitored, and the normalized decay is fitted to determine the carrier lifetime of the material. The decay dynamics shows a biexponential behavior with two characteristic timescales, namely a short lifetime and a long lifetime.

Results

The short lifetime of different Au dose series and different ion implantation energies are compared to determine the best way to fabricate hyperdoped silicon.

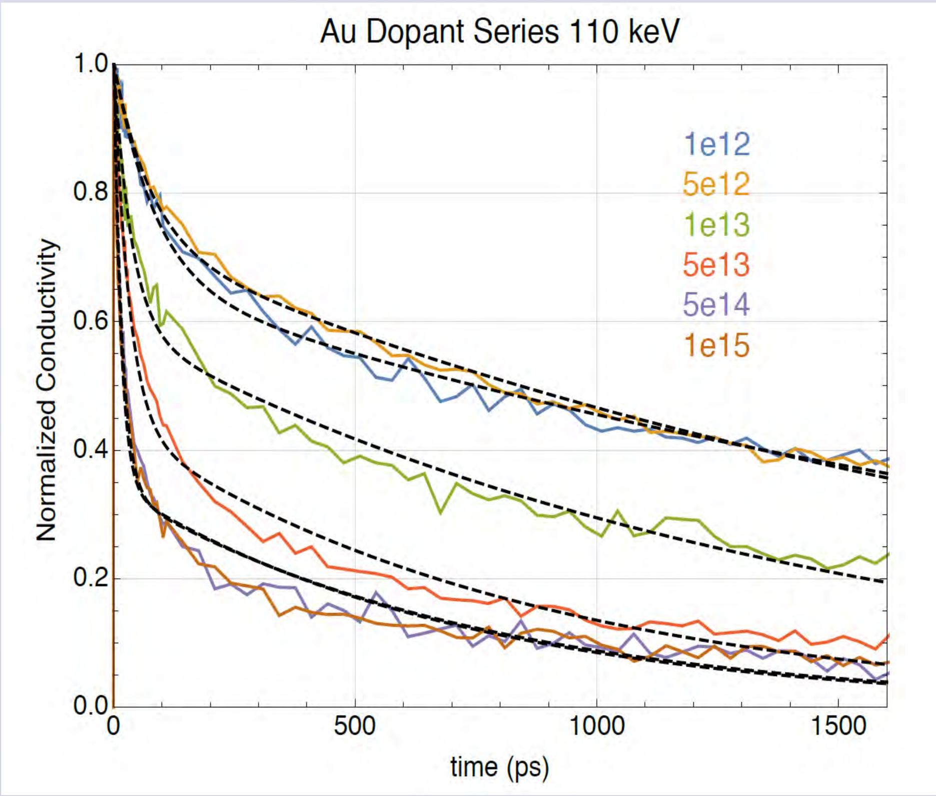

Figure 5 - Si:Au series with ion implantation energy of 110 keV and the PLM fluence of 0.8 J/cm^2

Figure 5 shows carrier lifetime decreasing with increasing gold concentration. The same trend is observed with dopants introduced at higher ion-implantation energy (Figure 6). The deep level dopants act as trap states, so Shockley-Read-Hall recombination rate is increased at higher dopant concentration.

Results continued

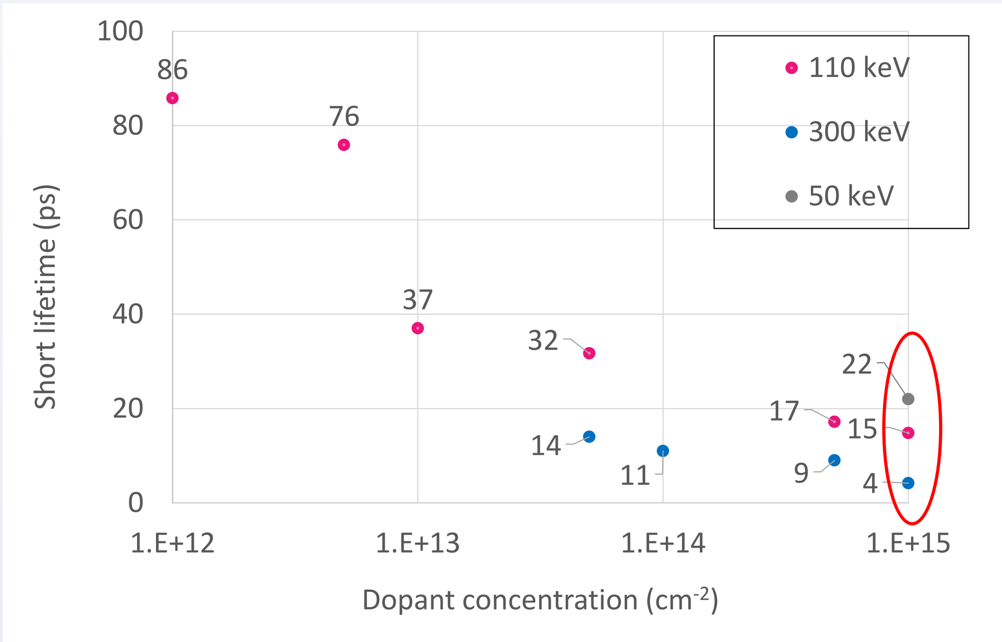

Figure 6: lifetime decreases with increasing Au dose as well as increasing implantation energy.

Moreover, at the same Au dose, the carrier lifetime decreases when the dopant is implanted at higher energy. A possible explanation is that the high implantation energy induces structural damage that is not removed by PLM.

The PLM process creates single crystalline hyperdoped material, but at the same time redistributes the dopant within the sample. As a result, dopant strongly segregate toward the surface. Figure 7 shows that the dopant is highly concentrated at the surface. At high concentration, cellular breakdown could occur during PLM process, leading to ununiformed lateral distribution of dopants. Figure 8 shows microscopic surface pattern after PLM. This could indicate cellular break down or other instabilities in the hyperdoping process. The structural imperfection could lead to shorter carrier lifetime.

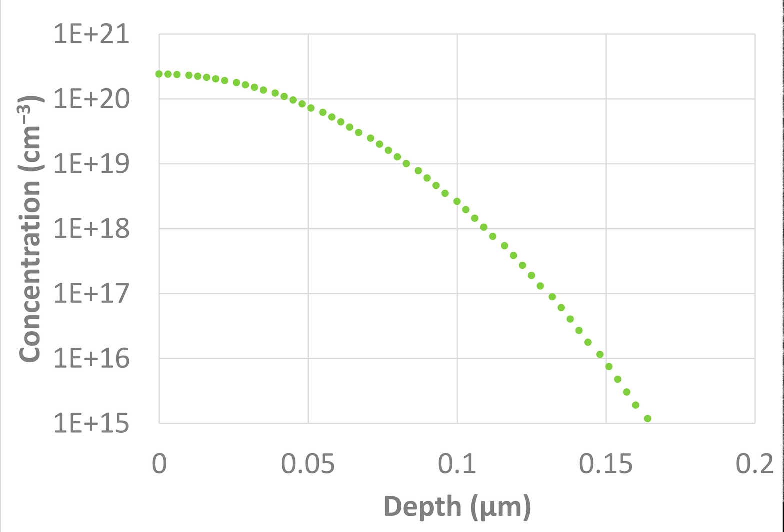

Figure 7 – Concentration profile of 1e15 Si:Au

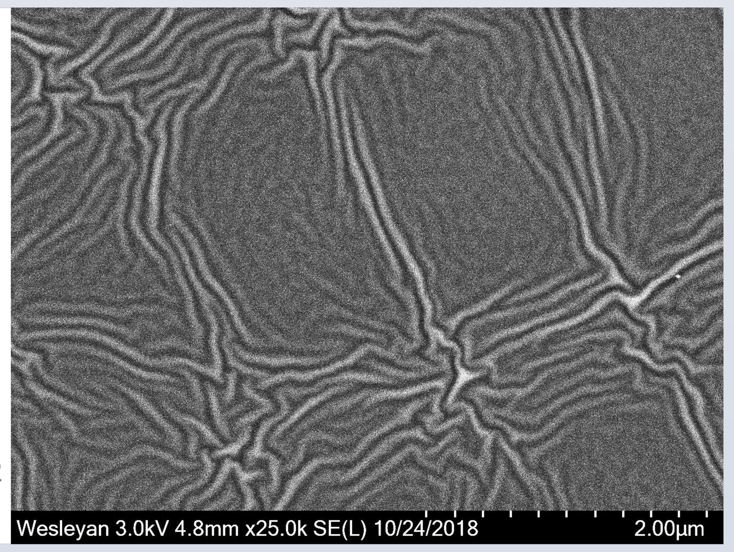

Figure 8 – Scanning electron micrograph of 50 keV 1e15 Si:Au

Conclusion

We use THz spectroscopy to study carrier lifetime in hyperdoped Si. We found that for Si:Au, the carrier lifetime decreases with

- increasing dopant concentration
- increasing ion implantation energy

This works sheds light on optimizing the hyperdoped material quality in order to achieve a high FOM.

References

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[2] Sullivan *et al.*, J. Appl. Phys. 114, 103701 (2013)

[3] Sher *et al.*, Appl. Phys. Lett. 105, 053905 (2014)