**Computational Modeling of Photoconductivity in Hydrogenated Amorphous Silicon for Sustainable Photovoltaic Applications**

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Abstract. This research aims to develop and numerically analyze a theoretical model describing photoconductivity in undoped hydrogenated amorphous silicon (a-si:h) under dual optical excitation. The main objective of the study is to establish quantitative relationships between the infrared (ir) illumination intensity and the steady-state carrier concentration, providing insight into charge transport mechanisms in disordered semiconductors. The research object is an amorphous silicon thin film, containing 5-8% hydrogen, which can be taken as a model of low cost thin film photovoltaic devices. In the simulation, equations for the generation, tunnelling relaxation, and localization-delocalization recombination of mobile carriers are solved numerically, and the results are used to calculate the population of localised states and the photoconductivity frequency dependence versus ir excitation intensity. The results show that the photoconductivity grows sublinearly with the ir illumination and that the delocalized carriers dominate at low temperatures (t < 50 k). As a result, both photoluminescence and photoconductivity spectra can be calculated simultaneously, yielding a unified picture of carrier dynamics in amorphous semiconductors that corroborates previously reported experimental findings and expands the understanding of defect-related transport in a-si:h materials. The results also suggest that hydrogenated amorphous silicon can be used as a stable and viable material for photovoltaics with the proposed model suitable for optimising devices, predicting long-term degradation behaviour, and for developing future thin-film photovoltaic devices.

**Keywords:** Amorphous silicon photovoltaics, Photoconductivity modelling, Dual beam illumination, Carrier kinetics, Numerical modelling, Sustainable energy materials, Thin film solar cells.

**INTRODUCTION**

**As the global identity of the energy sector pivots toward sustainable energy sources, photovoltaics (solar panels) are one of the most promising and fastest-growing routes for renewable energy. A successful photovoltaic future is dependent on material development that is low-cost and low-environmental impact at high efficiency. Thin-film semiconductors, such as hydrogenated amorphous silicon (a- Si:H), are well suited for large area coating, low temperature processing and flexible substrates [1, 2]. Although c-Si cells dominate the PV market today, thin-films will inevitably play an important role in future generations of solar cells and tandem devices, where flexible, lightweight or inexpensive substrates are required [3, 4].**

**Hydrogenated amorphous silicon is an unique material in which the disordered state and the presence of hydrogen atoms combine to reduce the defect density and increase the photoconductivity via hydrogen passivation of dangling bonds. The bandgap of 1.6 to 1.8 eV suits well for sunlight [5-6]. Due to the absence of long-range order, there exist localised states in the mobility gap. These states are important for charge generation, recombination, and transport in these materials. How these states interact with photocarriers is responsible for a number of the observed properties of amorphous silicon, such as the Staebler-Wronski effect, light-induced metastability, and shortened carrier lifetimes, and understanding the effect of these localised states on photocarrier dynamics is critical to the improvement of the performance and stability of a-Si:H devices.**

**The advent of new computational and experimental methods has vastly improved our understanding of defect physics in a-Si. New high-level atomistic simulation methods, such as machine-learning-based interatomic potentials, allow for the study of realistic a-Si:H structures with millions of atoms to quantitatively probe the formation and distribution of localised electronic states [10, 11, 12]. Interband generation, trap-assisted capture and emission, band-to-band tunnelling transitions and recombination are also increasingly being described using advanced kinetic and numerical models to analyse steady-state and time-resolved transient photoconductivity data [7, 13], as well as to help optimise deposition conditions, hydrogenation, and device designs.**

**Dual-beam optical excitation (visible (interband) and infrared (IR) radiation) has also proven to be an especially useful experimental tool for the studies of charge transport in amorphous semiconductors, via the generation of electron-hole pairs by visible-light and the photo-excitation from localised states into extended bands by infrared photons [14-16]. The inclusion of IR-induced excitation within models also provides a direct connection between the microscopic defect states and the responses that can be measured at the macroscopic level, such as photoconductivity and photoluminescence spectra.**

**Hydrogen can passivate deep traps but also creates metastable defects that induce light-induced degradation. It has been shown that controlling the amount of hydrogen incorporated during deposition in a PECVD reactor improves the stability and decreases the density of recombination centers [11]. Such improvements are vital for both reliability, and to meet modern PV manufacturing sustainability objectives due to the reduction in both represented energy and associated environmental impacts.**

**This article seeks to develop and numerically investigate a model for the steady-state photoconductivity of undoped (intrinsic) hydrogenated amorphous silicon (a Si:H) excited by dual-beam (visible + IR) illumination.** The model describes carrier generation, tunneling relaxation, and recombination within localized states while accounting for IR-induced photo-excitation into extended bands. By combining physically realistic density-of-states parameters with kinetic balance equations, this work provides a predictive framework for understanding and optimizing the photoelectronic behavior of a-Si:H thin films.

1. Formulate the system of balance equations for carrier generation, tunneling, and recombination including IR-induced transitions.
2. Implement a numerical simulation of steady-state carrier populations and photoconductivity as a function of IR intensity.
3. Compare calculated results with experimental data and previously published numerical studies.
4. Identify implications of the model for optimizing hydrogenation, minimizing defect density, and enhancing the efficiency and sustainability of a-Si:H-based photovoltaic devices.

# Theoretical model

In the present work, the photoconductivity of an undoped amorphous semiconductor is theoretically investigated in a two-beam technique at low temperature, when tunneling jumps of photocarriers upward in energy can be neglected. In constructing the theory, the results of work [4] are used, in which the distribution function  of localized photo-carriers generated during stationary interband optical excitation of an amorphous semiconductor was calculated. The notation of [4] is retained here: l is the type of carriers (electrons or holes), is the binding energy measured from the corresponding mobility limit, *R* and *r* are the distances from a given localization center, respectively, to the nearest localized carrier of a different type and to the nearest unfilled localized state with a higher binding energy . We will calculate the change in the distribution function of photocarriers, photoluminescence and photoconductivity arising as a result of exposure to IR radiation (also stationary). The absorption of this radiation causes photoexcitation of localized photocarriers into delocalized states, followed by their rapid recapture into one of the localized states and energy relaxation in these states, completed by radiative recombination with a carrier of another type or another emission into the zone of delocalized states. It is assumed that the energy of the IR quantum *hω*’ exceeds the binding energy for the overwhelming majority of localized photocarriers, and the dependence of the photoexcitation time  on the carrier binding energy (*I*’ is the IR illumination intensity) is neglected. In this case, it is possible to introduce a common reaction radius *RN* for carriers, determined from the condition

 (1)

where *T*l is the time of arrival of a particle of radius *R*N in a sphere, recombining with a particle of type l located in the center of the sphere. In what follows, for the sake of simplicity of presentation, the zone and kinetic parameters for electrons and holes will be considered identical. In this case, Te = Th = T, T’e = T’h = T’ and

 (2)

In this case, the balance equation  for the concentration of long-lived carriers can be represented as

 (3)

where G is the rate of interband generation of photocarriers. The differential rate of generation *G*(ɛ) into localized states with binding energy ɛ is determined by the expression

 (4)

which differs from that given in [4] by replacing G with the sum *G* + Δ*G*. Here Δ*G* is the rate of IR excitation of carriers from localized states to delocalized ones:

 (5)

g(ɛ) is the energy density of states, *p*(ɛ) is the concentration of unoccupied states with a binding energy greater than *ɛ*, ωo(*ɛ*) is the probability of a particle in state ɛ making a tunnel jump downwards in energy. The distribution function *f* is related to Г(ɛ)=G(ɛ)/[g(ɛ) – n(ɛ)] by the relation

 (6)

where *τ*(*R*, *r*) is the lifetime of a particle in the state (*R*, *r*),

(7)

*t*(r) is the tunnel relaxation time, τ(*R*) is the recombination time of the electron-hole pair. The reaction radius is given by another balance equation, which for a symmetric system of electrons and holes is reduced to the equality of the total rates of generation of short-lived and long-lived recombining particles,

(8)

where ω-1(ɛ) and ω1(ɛ) are the probabilities of a particle in state ɛ to recombine with a particle produced at a previous or subsequent time. The relations linking the probabilities ωs(ɛ) (s=±1;0) with the distribution function of localized carriers by energy are given in [4].

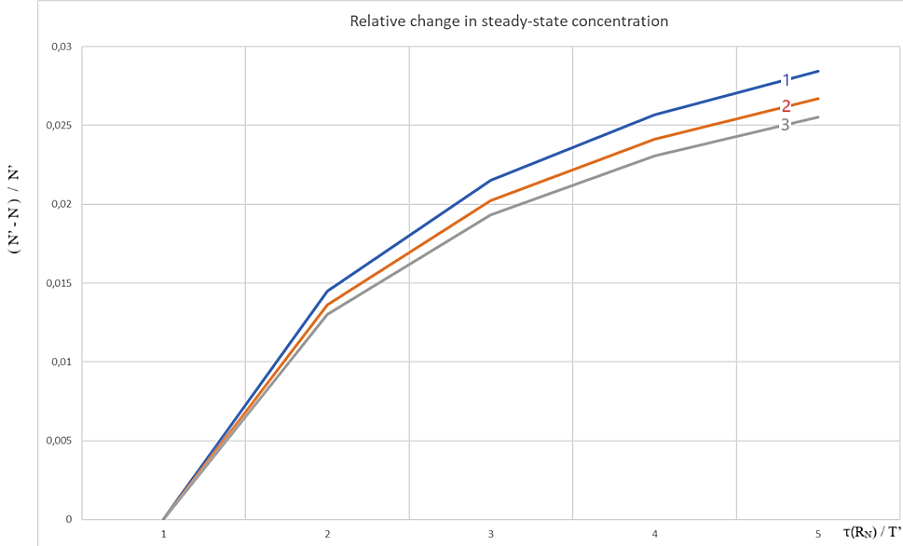
# RESULTS OF NUMERICAL CALCULATIONS

The change in the concentration of photocarriers as a result of using an additional infrared light source, also stationary, was considered in [5]. The relative change in the stationary concentration of localized photocarriers, the population of energy states g(ɛ)/n(ɛ), and its change depending on the intensity of IR radiation were calculated numerically. The photoluminescence and photoconductivity spectra in the two-beam stationary illumination method provide extensive information on the physical properties of the substance under consideration. In this paper, the frequency spectrum of photoconductivity was calculated numerically depending on the intensity of IR radiation.

For convenience, the abscissa axis shows not I’, but the ratio τ(RN)/T’ ~ I’. The concentration of steady-state excited carriers is N = : 5⋅1016 cm-3; 1⋅1017 cm-3; 2⋅1017 cm-3; curves 1, 2 and 3, respectively.

Figure 1 shows the dependence of the relative change in the steady-state concentration  on the intensity of the IR illumination I’. For convenience, the abscissa axis shows not I’, but the ratio τ(*R*N) / T’ ~ I’. Here N’ is the concentration taken for normalization and *R*N is the reaction radius for interband generation *G* in the absence of IR illumination. For sufficiently small values of I’, at which τ(RN)/T’ << 1 , the difference N’– N increases linearly with increasing I’:

(9)



**FIGURE 1.** The dependence of the relative change in the steady-state concentration (N’ - N) / N’ on the IR illumination intensity I’ is shown.

where the coefficient æ at G = 2.4⋅1019sm-3 s-1 [N0 = 1017sm-3, τ(*R*N) = 4.2⋅10-3s] is equal to 0.3. To estimate the time *T*’, one can use the expression for the time of photoexcitation of an electron from an impurity level, characterized by the binding energy *E*i, and the localization radius ɑ to the conduction band of a crystalline semiconductor, characterized by the effective mass *m*\*:

(10)

where λ = [( hω – Ei ) / E’]1/2 , E’ = h2 / (2m\*ɑ2) , *c* is the speed of light, nω’ is the refractive index at frequency ω’. At hω’ = 0.3 eV , nω’ = 3, m\* = m0 (mass of a free electron), ( hω’- Ei ) / E’= 6 we obtain T’ = 10-2 I’-1s ( I’ in Vt/sm2).

The photoconductivity current is contributed by delocalized carriers *j*1 = eGτµE (τ is the lifetime, µ is the mobility) and localized carriers *j*2 performing tunnel jumps down in energy in the electric field *E*. Experimentally, the contributions *j*1 and *j*2 can be separated by measuring the kinetics of the photocurrent after turning off the photoexcitation *G*: if the current *j*1 decreases in a microscopic time <10-12 s, then the decay time of the current *j*2 is comparable with the time τ(*R*N). With IR illumination, the current *j*1 increases by a factor of (G+ΔG)/G. The initial relative change in this current Δ*j*1/j01 = N0 / (TG) over a time of the order of – τ(*R*N) after turning on the illumination goes to a steady-state value

(11)

sublinearly dependent on the intensity I’. The calculation of the current *j*2, carried out according to formula in [4], gives at τ(*R*N)/T’<<1

(12)

where æ ~1 at *G* = 2.4·1019sm-3s-1.

# CONCLUSION

The other mechanism is carrier generation and carrier relaxation involving tunnelling, photo-excitation by infrared radiation and recombination. A quantitative approach based on a system of balance equations, including these processes, leads to a consistent microscopic picture of the mechanism of photoconductivity in disordered semiconductors. The simulation predicts two regimes for the variation of the photoconductivity with the IR intensity: a linear regime dominated by trap depopulation effects, and a sublinear saturation regime dominated by trap filling and recombination. The model also provides excellent agreement with the results of earlier and recent experiments, validating the reaction-radius and tunnelling-relaxation model for localised carrier dynamics. The energy redistribution of trap states under the IR illumination provides the mechanism of the observed enhancement in carrier mobility and decrease in activation energy, subsequently resulting in an increase in conductivity at low temperatures. The photoconductivity response is mainly affected by the concentration of hydrogen and defect density.

The optimised hydrogenation allows to avoid the introduction of deep-level defects and to improve the steady state conductivity. A large amount of hydrogenation leads to the formation of metastable complexes which in the long run can become detrimental, in agreement with the experimental evidence regarding the role played by PECVD and post-deposition treatments. From the sustainability viewpoint, the underlying computational model presents a high potential for optimising a high-performance photovoltaic device based on a-Si:H technology. The observed photoconductivity under bi-wavelength illumination is also useful to improve solar energy conversion in thin film devices. The model can connect light soaking, defect dynamics and hydrogen incorporation with changes in conductivity, enabling the rational design of green and durable solar cell materials. Future work will focus on experimentally verifying the predicted IR assisted transport phenomena, combining the model with multi-scale simulations of structural and thermal degradation, and acting as a foundation for sustainable manufacturing technologies. These efforts will bring amorphous silicon to the next generation of solar technology and our broader efforts in resilient, low-carbon energy systems of the future.

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