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An Open Source Based Repository For Defects in Silicon

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***Abstract* — Silicon is the most studied semiconductor, having almost every aspect of it being investigated. All this information is spread over a large set of publications, review articles and textbooks and cannot be found in a single location. Furthermore, the available data is not always consistent and depends on the techniques and samples used. This problem even exists for more specialised areas such as the study of defects in silicon photovoltaics, which is the focus of this paper. Currently, if a signature of a defect is experimentally determined a literature search must then be performed through texts going back decades in the hope to find a defect with similar properties. This paper addresses this time consuming activity by introducing an open source text based repository, which anyone can access or contribute to, and that provides clearly arranged information about defects in silicon.**

***Index Terms* — semiconductor impurities, database, photovoltaic cells, silicon.**

I. Introduction

Currently, silicon photovoltaic material is limited by bulk defects. However, many of these defects are unknown to the photovoltaic community, and an enormous amount of research is focused on both determining, and mitigating their effects on the performance of both solar cells and modules. This has resulted in a lot of effort searching through literature for defects and their impact. The lack of an easily accessible and well organised repository for this information has resulted in this process being performed by every research centre and almost every author that focuses on silicon used in solar cells. This paper aims to reduce this burden now and in the future by introducing a repository hosted online, that is open source and text based. The hope is that such a repository will both optimise future searches through literature, saving valuable time, and help direct research by allowing identification of holes in knowledge and these gaps to be subsequently filled. This paper provides awareness about this repository, it outlines the current scope, its specific terminology, and provides examples of how it can be used. It may furthermore be an ideal basis to identify contradicting experimental insights or conflicting data.

Historically, repositories have taken the form of engineering and scientific handbooks [1]–[4]. However, such repositories are static and closed systems by definition, do not support community-based maintenance, nor allow the information contained within them to be quickly extracted and used with other software or interfaces. If a database has been created, it is often left to an individual to maintain and allow others to access it [5]. This causes severe issues for longevity, especially as research contracts are typically only 3 years long. Recently, other areas of research have started embracing open access repositories for storing and sharing data. One such example is the work of Mikhail Polyanskiy [6], [7], who is continuing the work of Palik [8] by tabulating the optical constants of different materials. This format has facilitated contributions for the optics community with the repository now containing records for over 200 inorganic materials, with almost 1000 entries, and over 50 organic materials. This format ensures that the repository can be: accessed into the future, continually contributed to, and the maintainer replaced at any time with ease. This example demonstrates the feasibility and interest in such repository systems for the scientific community.

This paper reports on the text based repository, currently hosted on GitHub, that contains information about defects in silicon. The paper will first provide a brief background on how defects behave in silicon, second outline the information that will be contained within the repository before finally providing an analysis of the limited data that is currently within the repository.

II. Background

Impurities or defects have been studied in semiconductors for almost as long as semiconductors have been known about. In fact, it is through the deliberate incorporation of certain impurities into semiconductors that has paved the way for the modern world. Impurities in semiconductors allow the conductivity of the material to change, the ability to form p-n junctions, to control the effective lifetime and hence the speed at which it can operate, and even change the absorption of the material.

Defects are a concern when they insert an energy level into a semiconductor's 'forbidden region', as shown in Figure 1. In the figure E_c is the energy level of the conduction band edge, E_v is the energy level of the valance band edge, E_i is the energy of the intrinsic level, E_d is the energy level of the defect, G is the elevation of electrons by any means, c_e is the capture of electrons from the conduction band into the defect, e_e is the emission of electrons from the defect into the conduction band, c_h is the capture of holes from the valance band into defect and e_h is the emission of holes from the defect into the valance band.

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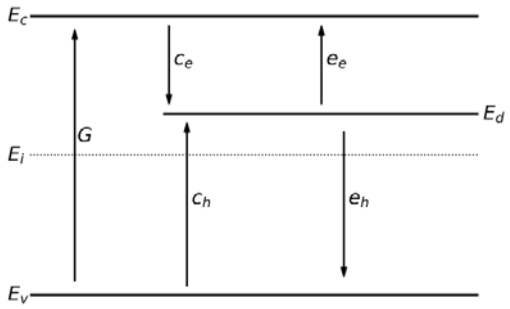

Figure 1: Basic energy level diagram showing the generation of free electrons and the possible exchanges with a defect level E_d.

A single level defect, such as above, can be completely described if its four rate constants, associated with the transition into and out of the defect, are known. Through the use of detailed balance, it is possible to show that such a system only requires three independent variables to describe the kinetics of a specific defect[9], [10]. These three values are the defect's energy level E_d, the capture cross section for electrons (σ_e) and the capture cross section for holes (σ_h)[9], [10]. Note that, these three variables should be assumed to be temperature dependent. If the concentration of the defect is known, the impact the defect has on the samples dopant concentration, carrier density with time, and hence lifetime [9]–[11] can be determined. It is the impact of these defects on the carrier lifetime, and hence the maximum voltage that is obtainable for a solar cell that is of primary interest for the authors. For this reason, this parameterization is to be captured within this repository. The following section will detail how this information is recorded and how it is ensured that the information can be accessed and/or contributed to by anyone at anytime.

III. Repository Details

The structure of a repository determines, how it can be accessed, how it can be changed, and eventually how often it is used. The information contained within this repository is held in the folder structure, file names, and in the text within the final ASCII based files. This format has been chosen as it allows:

a. Browsing of the repository without the need of any program, or interface, e.g. a word, spreadsheet or database program.
b. Future proofing of the repository by not conforming with a specific database language.
c. Operating system and platform independent.
d. With defined rules simple scripts can be written to change the plain text database into a conventional database, e.g. SQL or csv.
e. The possibility of future implementation of graphical browsing skin/application.

The folder structure of the repository is intended to be both easy to navigate, add and edit data. We will first outline the folder structure and file naming conventions before providing a detailed example for a specific defect. A scematic of the fold and file structure is shown in Figure 2. The highest folder in the repository represents the material that the defect is in, i.e. for the current scope, the host material is silicon and so "Si" is the highest folder. The next level of folders represents elements that constitute the defect. Inside this folder are plain text files that contain the specific information about the defect. If a defect consists of more than one element, the information will be duplicated in different files in under each respective element. The plain text files have an "srh" extension, to highlight that they contain the Shockley Read-Hall parameterisation of a defect. However, these "srh" are saved as plain text documents written with YAML syntax, and as such can be read by any text editor. There is a separate file for every unique charge state of a defect. The text files are named to allow unambiguous identification of defect they contain. The naming convention used is as follows. There are three distinct parts to each name separated by underscores (_). The first part of the name contains all the elements that constitute the defect. The first element is the element within the folder, followed by an alphabetical listing of the other elements. The second part of the name contains hyphen separated (-) terms that indicate how the associated element sits in the crystal lattice, i.e. 'i' stands for the element is as an interstitial and 's' is for substitutional. The final part of the name defines the charge state of the defect, i.e. donor (d), acceptor (a), double donor (dd), double acceptor (da). A donor type defect can either be neutral or donate an electron. If the electron is donated the defect positively charged.

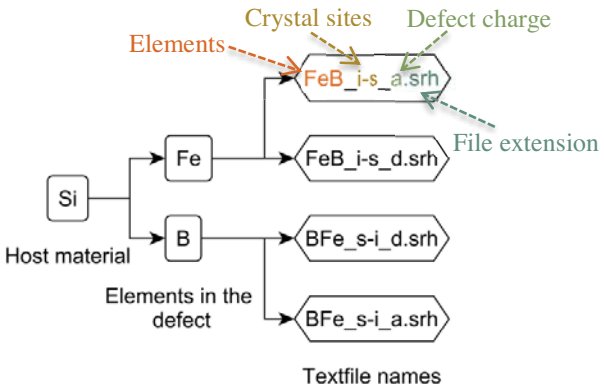

Figure 2: Folder and file structure used in the repository for the Iron Boron defect. Square boxes represent folder levels, while hexagons represent the final plain text file.

For the sake of clarity, an example of the folder structure and file naming convention for the well known Iron-Boron defect in Silicon is provided, the same example as if Figure 2. As the host material is Silicon, the highest level folder is "Si". In side this folder are all the elements that constitute the defect. The elements which constitute this defect are Iron and Boron. Thus, the information about this defect (held in the plain text documents) are found in both the "Fe" folder and in the "B" folders. Within both these folders exists the same information about the defect. Within the "Fe" folder the files:

"FeB_i-s_d.srh" and "FeB_i-s_a.srh" exist. Note that the files are ASCII files, and the file extension, ".srh", is solely to reflect that these files contain Shockley Read Hall defect parameters. As is evident from the first part of the file name, this defect contains two elements, iron and boron, shown in Figure 2 in orange. The second part of the name, shown in Figure 2 in yellow, provides that the iron atom is in the silicon as an interstitial atom, while the boron atom has substituted a silicon atom in the crystal site. Finally, the last part of the file name, shown in Figure 2 in light green, shows why there are two different files, i.e. the iron boron defect has two different energy levels, the first acting as a donor level and the second as an acceptor level, respectively.

The plain text files also contain a significant amount of information. Within the files is listed different publications that have contributed defect parameters about that specific defect. The publications are referenced using a unique id, being an author-year notation. For example, in the current "FeB_i-s_a.srh" file you will find an entry for "Graff1995". Here the last name of the first author of the publication is Graff and the publication year was 1995. When there are several publications from authors with the same last name in the same year, letters are appended to the end of this id to form a unique id. If an author provides several different values for the same defect in the same publication, the author name is appended with an underscore and then a number, e.g. Graff1995_1. Under this title the following information is captured: "title", the title of the publication; "DOI", the digital object identifier; "measurement_technique", a comma seperated list of measurement techniques used in the paper to obtain the values; "comments", additional comments that may be helpful; "sample", an optional field setout in a similar manner to params detailing with information about the samples used in the publication; and finally "params", contains the Shockley Read Hall parameterization of the defect including error values.

The Shockley Read-Hall parameters captured are: "Ed" the energy level of the defect, "simga_e" the electron capture cross section, "sigma_h" the hole capture cross section, and "k" the ratio of the capture cross sections. k is captured as this is the value directly measured in lifetime spectroscopy, and thus allows easy entry into the database without the assumption of capture cross-sections from other publications. The energy level of the defect is usually measured relative to the conduction band edge, or valence band edge. These values are thus recorded as "Ev+0.38". To record a full set of the three parameters the temperature dependence needs to be included. This temperature dependence is recorded using standard scientific notation, e.g. the temperature dependence of σ_h for interstitial iron acting as a donor is recorded under "sigma_h" as "3.9e-16 * exp(-0.045/kT) "[12].

Published errors on these values are also able to be captured. An error is recorded in the repository by creating a new field under the "params" where the key is the parameter in question with a "d" appended as a prefix, e.g. the error in E_d is recorded under dE_d. Symmetric error values are recorded through listing a single number, while asymmetric errors are comma separated starting with the negativity error value. For example, to enter the error Diez [13] reports for Cobalt's acceptor capture cross-sectional ratio (k) being -0.1 and +0.53, it is entered under the dk as "0.1, 0.53".

IV. Analysis

At the time of publication, the repository has 235 entries covering 83 unique defects, representing a total of 131 different defect charge states[1], [3], [12]–[29]. Of these only 16 different defect charge states have information for the three required parameters being the energy level, hole capture cross section, and electron capture cross section. It is expected that in the following year this list will dramatically increase. With this data available we can investigate the common assumption that deep defects, defect located close to E_i, have the largest impact on sample lifetime.

To investigate this, the 16 charge states that have a full set of parameters were taken and the lifetime for each level determined as if they were independent of each other [9]. The lifetime was calculated for two different samples being: a p-type sample doped with 1×10^{16} cm^{-3} atom, and a n-type sample doped with 6×10^{15}. The excess carrier density was set to 1×10^{13} cm^{-3} and each defect was assumed to have a concentration of 1×10^{13} atoms per cm^{-3}.

The lifetime as a function of the defects state level is shown in Figure 3. The defects are observed to have approximately the same recombination strength, except for the donor level of Nickel which is very recombination active, and the acceptor level of Cobalt and donor level of iron which are not very recombination active. The same data can also be displayed as a function of the defects' energy level from the intrinsic level, as shown in Figure 4. Along with the effective lifetime of the minority carrier in doped samples is shown the mean carrier lifetime if a defect is completely occupied by the other carrier, i.e. the lowest lifetime possible for that carrier. No general trend can be observed in this data set for the recombination strength of defect as a function of energy level. However, this dataset is rather small. It is the hope of the authors that as the repository becomes more complete, such analysis will be able to be performed with a higher degree of accuracy.

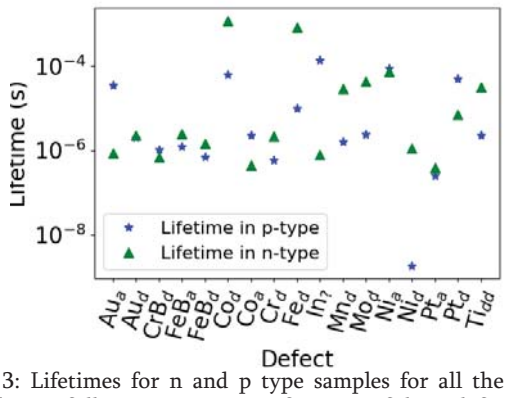

Figure 3: Lifetimes for n and p type samples for all the defects which have a full parameter set as a function of those defects.

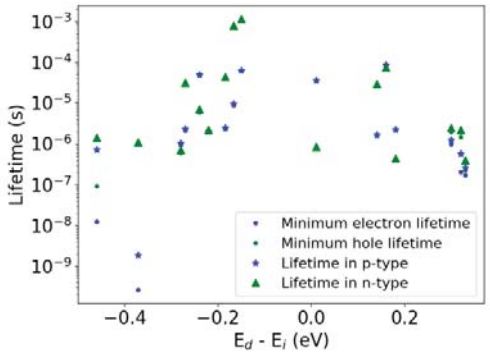

Figure 4: Lifetimes for n and p type samples for all the defects which have a full parameter set as a function of the energy level. Also displayed are the minimum electron and hole carrier lifetimes possible.

V. Conclusion

We have presented an open repository that shall contain the Shockley Read-Hall parameterisation of defects. The format of the defects has been outlined, and an example analysis of the data has been provided. The open-access repository can be constantly updated and is independent of any specific program or interface. It does not require a specific person or institution for maintenance. The repository can greatly help solar researchers finding and analyzing defect data and the corresponding publications.

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