

Luminescence: science and applications in silicon photovoltaics

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In nature, nearly every material has its unique luminescence footprints. These footprints are strongly dependent on material properties, device structures, surrounding environments, and measurement conditions. These complex relationships provide us with unique opportunities to explore the properties of photovoltaic materials and devices by performing luminescence measurements just from above the sample surfaces. A silicon solar cell can emit many luminescence peaks under appropriate excitation conditions. By investigating the fundamental properties of these peaks (energy, shape, and intensity) and their evolutions versus various fabrication and measurement conditions, we can extract many critical properties of the solar cell. This extended paper presents the physics and our recent advances in luminescence spectroscopy and imaging techniques to characterize silicon wafers and solar cells.

Introduction

In simple terms, luminescence in a semiconductor is the emission of photons from the material when electrons from higher energy states make transitions to lower energy states. In crystalline silicon (c-Si), the luminescence phenomenon consists of both band-to-band and deep-level luminescence. The band-to-band emission is due to radiative transitions of free electrons in the conduction band to empty states in the valence band, and it reflects the intrinsic properties of Si. On the other hand, the sub-bandgap emission is due to the radiative recombination of electrons and/or holes trapped by defect and impurity centers occupying energy levels inside the Si band gap, and thus it reflects the properties of defects and impurities within the host material. These schemes are illustrated in **Fig. 1a**. Although the luminescence signal is emitted by the material itself, the luminescence spectrum detected outside the material is a complex combination of numerous phenomena which are both intrinsic and extrinsic to the material properties. Luminescence spectra from c-Si wafers are determined by (i) the material properties; (ii) the energy and power of the excitation source, and the surface recombination. These properties determine excess carrier profiles inside the silicon wafers, which generally affect the luminescence spectral shape; (iii) the optical properties of the wafer surface, which determine the escape probability of the generated photons; and (iv) the spectral response of the optical equipment employed to capture the luminescence signal. This paper provides a theoretical background on the luminescence phenomena from c-Si wafers from a physical point of view. It also exploits the rich information embedded in the captured luminescence spectra and demonstrates a wide range of applications for Si photovoltaics.

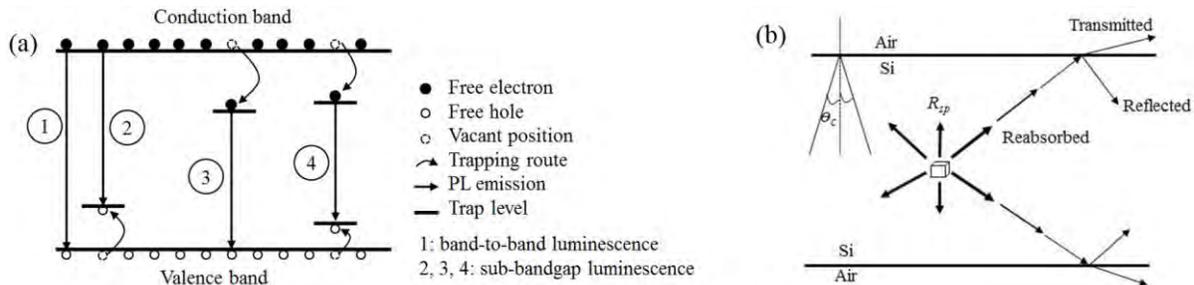


Fig. 1: (a) Illustration of luminescence schemes in c-Si wafers. (b) Loss mechanisms of spontaneously generated photons inside a c-Si wafer. Note that the incident, reflected, transmitted and critical angles in this figure are not presented in actual scales.

Application 1: Establishment of fundamental properties

According to the generalized Planck law (Würfel et al., Appl. Phys. A 60, 67 (1995)), the spontaneous photon flux per energy interval emitted from a volume element of a certain semiconductor under excitation into the entire hemisphere is given by:

$$R_{sp}(\hbar\omega) \propto \alpha_{BB} \times (\hbar\omega)^2 \times \exp\left(-\frac{\hbar\omega}{kT}\right) \times \exp\left(\frac{\Delta\mu}{kT}\right) \quad (1).$$

$\Delta\mu$ and α_{BB} are the chemical potential under excitation and the absorption coefficient of c-Si, respectively. After the photons are spontaneously generated, to escape the semiconductor, they have to overcome two loss mechanisms illustrated in **Fig. 1b**. First, these photons have to survive reabsorption on the way to the wafer surface. The reabsorption is characterized by α_{BB} . Second, the photons have to arrive at the surface at an incident angle which is smaller than the critical angle θ_c . Otherwise, they will be totally reflected back and do not have any chance to escape. At the surface, after the reabsorption, the remaining

photons within the critical angle can be either reflected back or transmitted into the outside environment. Accounting for these phenomena, the photon flux emitted from a c-Si wafer is then given by:

$$PL = \left[\int_0^w \frac{R_{sp}}{4n^2} \times \exp(-\alpha_{BB}x) dx \right] \times A \quad (2),$$

where w is the wafer thickness, n is the refractive index of Si, and A is determined by the geometry and internal reflectivities on both wafer surfaces.

Based on (1) and (2), at a given temperature, if the excess carrier profile and surface optics are well controlled, the values of α_{BB} can be extracted accurately from the spectrum captured, as shown in **Fig. 2a**. From α_{BB} values, the temperature dependence of the radiative recombination coefficient B can also be determined (**Fig. 2b**).

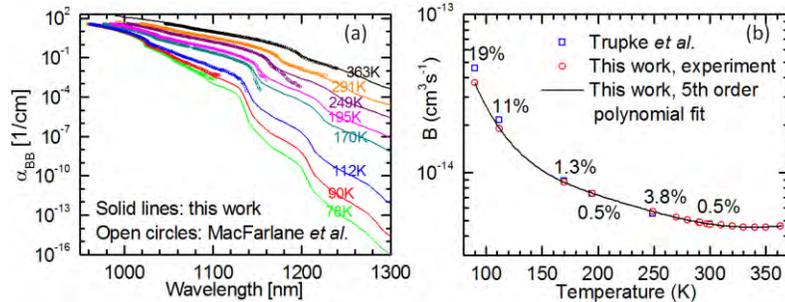


Fig. 2: (a) α_{BB} and (b) $B(T)$ of crystalline silicon obtained from PL at different temperatures in this work (J. Appl. Phys. 115, 043710 (2014)) in comparison with data from MacFarlane *et al.* (Phys. Rev. 111, 1245 (1958)) and Trupke *et al.* (J. Appl. Phys. 94, 4930 (2003)). The inserted numbers are the relative deviation between the two works.

Application 2: Characterization of heavily-doped layers and surface passivation films

When different layers of various materials are stacked together, if we employ an appropriate excitation wavelength, the excitation light will be absorbed in all layers. Each of these layers will then emit its own photoluminescence (PL) spectrum. Since different materials have their unique bandgaps, absorption coefficients, and radiative recombination mechanisms, the PL spectrum emitted from each layer is distinct. Therefore, the total spectrum captured contains signatures of all layers. For example, in **Fig. 3a**, the P1, P2, and P3 peaks correspond to the SiN passivation film, c-Si substrate, and diffused layer, respectively. Utilizing peak P3, we can map sheet resistances of locally-doped fingers in various interdigitated back contact (IBC) solar cells with ultra-high spatial resolution (**Fig. 3b**). Meanwhile, the P1 peak intensity is directly related to the SiN film thickness. Thus, we can convert its intensity image, captured with a PL imaging tool and a 600-1000nm band-pass filter, into an absolute thickness image (**Fig. 3c**).

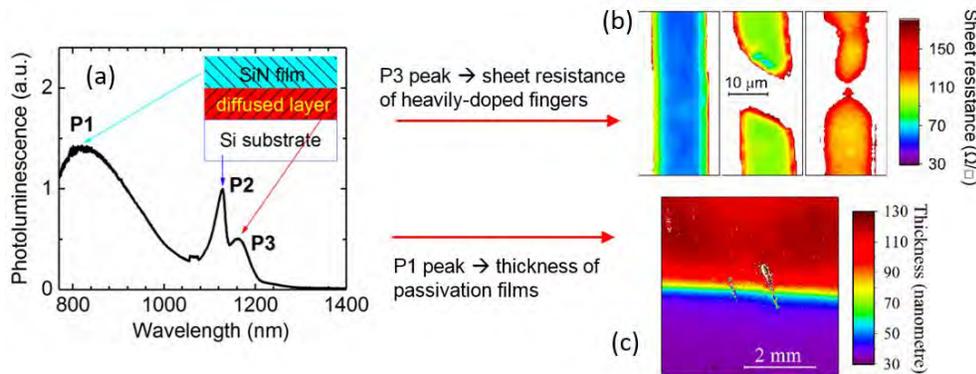
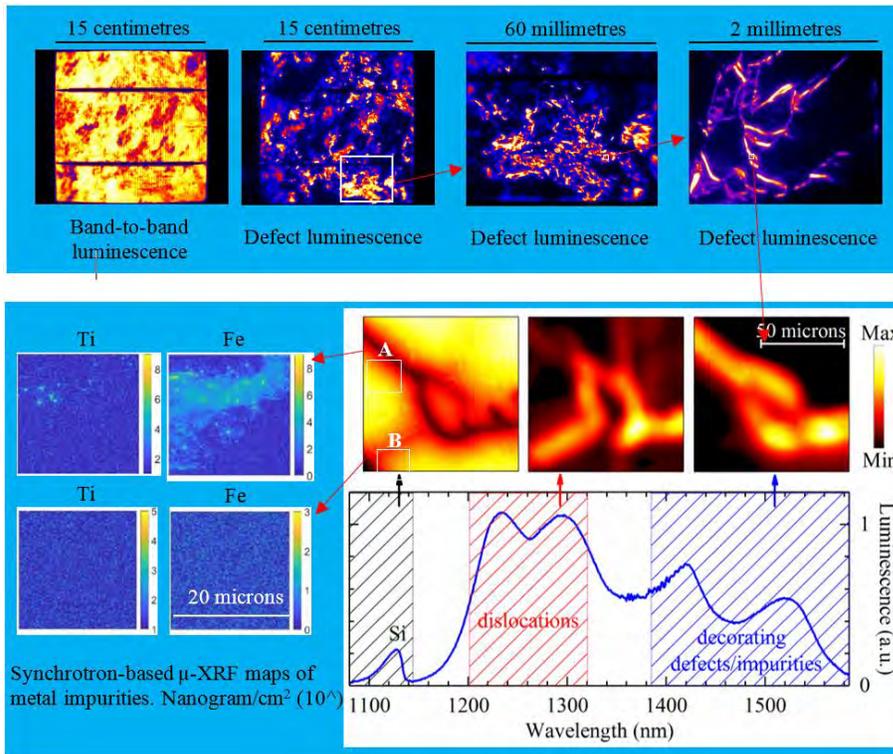


Fig. 3: (a) Total PL spectrum from a stack of various layers. (b) Sheet resistance maps of IBC solar cell fingers, using peak P3. (c) Thickness imaging of passivation films, using peak P1.

Application 3: Multi-scale characterization of defects and impurities in c-Si wafers

A very powerful approach for device improvements is the linking of micro/nano-scale material and device properties to macro-scale device performances. Combining both luminescence spectroscopy and imaging, we can unlock physical mechanisms of how extended defects and impurities can affect the overall performance of real working solar cells. For example, band-to-band and defect luminescence imaging allows us to pinpoint to the location of extended defects (top cluster in **Fig. 4**). The luminescence spectrum then can reveal signatures of various recombination centers, allowing very high spatial resolution maps of these centers (bottom cluster in **Fig. 4**). From the three luminescence maps (bottom cluster in **Fig. 4**), we can conclude that the trapped defects/impurities around dislocations are more detrimental in terms of recombination activity than the dislocations themselves. Also, using spatially-resolved synchrotron-based micro-X-ray fluorescence measurements, we confirm that high densities of metal impurities are present at positions with strong emissions from decorating defects/impurities.



Top: luminescence imaging for fast diagnostics

Fig. 4: Combining PL imaging (top cluster) and PL spectroscopy (bottom cluster) for both band-to-band and defect luminescence, we can deeply understand impacts of various defects and impurities on the material quality.

Bottom: In-depth analysis of micro-features, combining both spectroscopy and microscopy

Application 4: Characterization of doped poly-Si films

Luminescence also offers many opportunities to explore, understand, and optimize passivating-contacts for solar cells based on poly-Si films. We have found that at low temperatures the films emit a characteristic broad luminescence peak at energies lower than the c-Si bandgap. Based on such phenomenon, we have demonstrated several applications to understand the behavior of poly-Si/SiO_x passivated contacts in terms of carrier recombination and transport: i) the films contain radiative defects whose energy levels continuously stretch from the band edges to deep levels inside the poly-Si bandgap (**Fig. 5b**) and ii) it is possible to detect hydrogen introduced in the passivating contact stacks by analyzing the luminescence emission from its partial amorphous phase (**Fig. 5c**). The discovery and investigation of luminescence phenomena from doped poly-Si films opens the door to access the optoelectronic properties of both the films themselves and the entire passivating structure in a very fast, contactless, and non-destructive manner. A range of applications stemming from this phenomenon are possible such as i) studies of carrier transport behaviors and defects inside the films, ii) hydrogenation inside the films for improving their passivation quality, and iii) time-resolved photoluminescence to extract carrier lifetimes in the films and the c-Si substrate separately by monitoring their corresponding luminescence peaks.

Summary

The captured luminescence signal is a complex combination of numerous phenomena occurring in both the silicon wafers and measurement equipment. The emitted spectrum itself is determined by the intrinsic properties of silicon, defects and impurities in the host material, experimental conditions, and surface optics. The detected spectrum is then affected by the spectral responses of the photoluminescence spectroscopy/imaging systems. However, viewed from a different perspective, these relationships are, in fact, opportunities for exploring potential applications of spectrally-resolved luminescence. By systematically controlling and monitoring the parameters which can potentially affect the detected spectra, certain properties of silicon wafers and solar cells can be evaluated. This extended presentation will exploit these complications and present up-to-date different applications of spectrally-resolved luminescence-based techniques for Si photovoltaics.

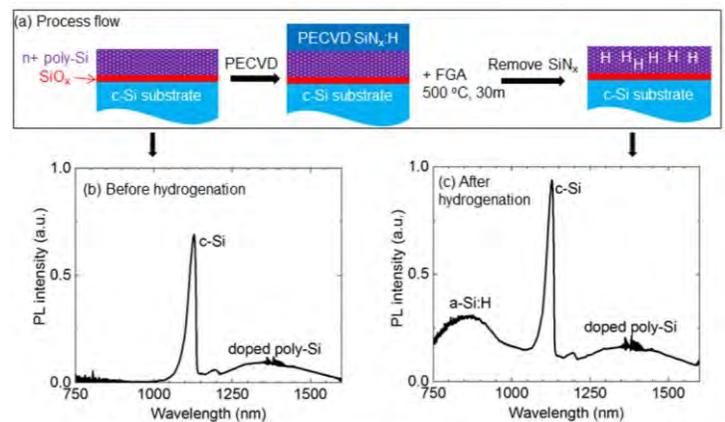


Fig. 5: (a) Process flow for hydrogenation. PL spectra (b) before and (c) after hydrogenation. $T = 80 \text{ K}$, $\lambda_{\text{exc}} = 405 \text{ nm}$.