Potential of Si$_{1-x}$Ge$_x$ alloys for Auger generation in highly efficient solar cells

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Abstract. Recent investigation on Si solar cells demonstrated the utility of Auger generation for the creation of more than merely one electron/hole pair per absorbed photon. The semiconductor Si requires a minimum photon energy of about 3.4 eV for this internal carrier multiplication. The current of a Si cell is therefore not significantly increased by Auger generation when the cell is illuminated by an air mass 1.5 spectrum, which contains only few photons with energies above 3.4 eV. Use of Si$_{1-x}$Ge$_x$ alloys promises a lower onset energy. Unfortunately, incomplete data on band structures of random Si$_{1-x}$Ge$_x$ alloys preclude a detailed quantitative discussion of the full potential for these materials. Nevertheless, (i) analogies to our own quantum efficiency data from pure Si, (ii) the calculated band structure of the hypothetical, ordered zincblende type Si$_{0.5}$Ge$_{0.5}$ crystal, and (iii) optical data for Si$_{1-x}$Ge$_x$ alloys indicate an optimum Ge content of $x = 0.6$ to $x = 0.7$.

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Quantum efficiencies in excess of unity were demonstrated for silicon solar cells [1], for photodiodes [2, 3], and for Schottky-barrier detectors [4]. Impact ionization by optically generated hot carriers is responsible for the creation of more than merely one electron/hole pair per absorbed photon. This inverse process of Auger recombination was termed as Auger generation [5]. Consideration of Auger generation led us to new upper limits for photovoltaic energy conversion: The ultimate efficiency [5] (neglecting any recombination) as well as the detailed balance limit [6] (including radiative recombination) increase substantially. For example, a solar cell which makes optimal use of internal carrier multiplication and with radiative recombination as the only loss mechanism has now a maximum possible theoretical efficiency of 43% (instead of 30% without carrier multiplication) for illumination by the sun's blackbody radiation [6]. However, useful Auger generation over a wide wavelength regime of the incident radiation requires specific band-structure features of the semiconductor [5, 6].

Demands on the band structure for a high potential of Auger generation were empirically concluded from observations at solar cells from Si [1, 5], in which photons with energies $h\nu \geq 3.4$ eV lead to optical transitions at distinct points in the Brillouin zone. Carrier multiplication by Auger generation then entails quantum efficiencies above unity. (The highest Internal Quantum Efficiency (IQE) observed was IQE = 1.3 [1].) Since the solar spectrum contains only very few photons in this regime, the maximum increase in the short-circuit current of a solar cell from pure crystalline Si under air mass 1.5 global illumination is below 0.5 mA/cm$^2$; elemental Si thus gains little in cell efficiency by carrier multiplication. The onset of Auger generation should hence be shifted to the wavelength regime of visible light, for example by reducing the fundamental band gap $E_G$ by mixing the semiconductor Si with Ge in order to form Si$_{1-x}$Ge$_x$ alloys. However, not only the fundamental band gap but the overall band structure has to be optimized towards effective Auger generation [5, 6].

The present contribution discusses the potential of Si$_{1-x}$Ge$_x$ alloys for internal carrier multiplication. The band structure promises quantum efficiencies above one in the wavelength regime of visible light. The optimum Ge concentration $x$ is determined from the requirement of a minimum onset energy for Auger generation; alloys between a minimum $x \approx 0.6$ and a maximum $x \approx 0.7$ seem most favorable.

1 Energy and momentum conservation

Creating two (instead of one) electron/hole pairs within a semiconductor of fundamental band gap $E_G$ requires
Fig. 1a, b. Detail of a band structure with lowest gap being indirect, allowing for a minimum onset energy of Auger generation. A photon (wavy arrow) is absorbed by a direct optical transition at energy $E_D = 2E_G$; (a) Onset of carrier multiplication due to relaxation of hot primary electron $e_t$, (b) onset due to primary hot hole $h_1$. In both cases, relaxation of the hot carrier towards the band extremum induces the creation of a secondary carrier pair $e_2/h_2$ across the fundamental gap $E_G$. The wavy arrow of the initial optical transition points towards the primary carrier which seizes the full excess energy, hence causes Auger generation.

Fig. 2a, b. Auger generation for positions $E(k)$ where both primary carriers $e_t$ and $h_1$ get an amount of excess energy. The carrier with the major part of excess energy relaxes towards the band edge via Auger generation: (a) carrier multiplication via a hot electron (1); and (b) multiplication via a hot hole (2).

Both cases, the primary carrier relaxes in a one-step-process towards the band edge and creates a secondary electron/hole pair $e_2/h_2$. The identical lengths and opposite directions of the dash-dotted transition arrows in Figs. 1a, b ensure the conservation of energy $E$ and momentum $k$. If the band structure of a semiconductor follows one of the situations described in Figs. 1a or b, a minimum onset of Auger generation at $hv = 2E_G$ is possible. However, efficient utilization of Auger generation in solar cells further requires that also higher photon energies are (i) strongly absorbed and (ii) lead to hot, Auger-active primary carriers.

Figures 2a and b show the Auger-generation processes if the primary excitation takes place at a $k$ vector where neither the conduction band nor the valence band reach extremal values. Figure 2a refers to carrier multiplication by a hot electron $e_t$ which is created via a direct optical transition at an energy $E_D > 2E_G$. In $E(k)$ space, this transition takes place at an energy of the valence-band edge which is an amount $\Delta E_V$ smaller than at its maximum. In the case of Fig. 2a, the primary hole $h_1$ obtains only an excess energy $E_{x,h} = \Delta E_V$ with $\Delta E_V < E_G$. The hole $h_1$ is therefore unable to generate secondary pairs. In contrast, the primary electron $e_t$ is able to excite a secondary pair if its excess energy $E_{x,e} > E_G + \Delta E_V$. This full amount of energy $E_{x,e}$ is needed since the excitation of the secondary pair has to take place across $E_G + \Delta E_{e1}$ instead of across $E_G$ only. The generation process of Fig. 2a with the hot electron $e_t$ is therefore