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# ENERGY BANDS CALCULATION IN NANOSTRUCTURED META-MATERIALS FOR SOLAR CELL APPLICATIONS

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## 1) Context / Study motivation

The use of nanostructures introducing a 1-D (ultra-thin layers), 2-D (nanowires) or 3-D (dots) quantum confinement can increase the conversion efficiency of the third-generation photovoltaic cells. The origin of such an increase is based on the improvement of absorption of the solar spectrum by varying the gap of the material in which the conversion between photon and electron/hole pair takes place. An innovative solution is to consider composite or meta-materials based on silicon (such as silicon nanocrystals embedded in a dielectric matrix, SiO<sub>2</sub>, SiON, SiC or Si<sub>3</sub>N<sub>4</sub>). These meta-materials involve a remarkable property of semiconductor nanostructures for which the material bandgap varies with the characteristic size of the system (quantum confinement) [1-7]. This bandgap engineering can be used in devices called "tandem solar cell", as that recently proposed in the literature [1, 3] (Fig. 1). The idea is to add one or more layers of nano-structured materials on the top of a solar cell for which the optical absorption covers different domains of the solar spectrum. These meta-materials offer the advantages of using silicon which is abundant, stable, non-toxic and capable to diversify in order to obtain both a medium bandgap (~1eV) and a high bandgap material (~1.7eV).

## 2) Description of approach

In this paper we propose a simple calculation of the energy band in nano-structured meta-materials based on ultra-thin periodic Si/SiO<sub>2</sub> layers (quantum-well superlattice) for third-generation solar cell application. For this purpose, the Schrödinger equation (with periodic Bloch's conditions) [8-10] is numerically solved considering the potential profiles of both the valence and conduction bands of the Si/SiO<sub>2</sub> system (Fig. 2). This method allows us to analyze the carrier energy band structure and to extract the essential electronic properties (bandgap, miniband width) of such meta-materials based on 1-D periodic nanostructures.

## 3) Results / Conclusions / Perspectives

Fig. 3 shows the carrier energy bands structure of the meta-material as calculated with our approach

for a Si layer-thickness  $L=0.75\text{nm}$  and a spacing  $H=0.75\text{nm}$ . The energy band structure is strongly modified compared to that of a single quantum well. For thin Si-layers positioned very close one to each other and separated by a finite barrier (as is the case for Si/SiO<sub>2</sub> barrier), a significant wave function overlap is obtained. This leads to the splitting of the discrete energy levels (below the maximum of the energy barrier) into minibands (as schematically illustrated in Fig. 2). The bandgap of the meta-material can be also calculated from the band structure of Fig. 3 considering the positions of the extrema of the first miniband, respectively for electrons and holes. This figure clearly shows a widening of the meta-material bandgap (2.667eV) compared to the bulk Si bandgap (1.1eV). Fig. 4 shows that the meta-material bandgap strongly depends on the thickness of the Si layer. The bandgap increases from 1.1eV for bulk Si to 3.45eV for  $L=0.5\text{nm}$ , due to a strong 1-D quantum confinement occurring in very thin Si-layers. Fig. 5(a) shows the calculated energy as function of the Si-layer spacing  $H$ , for  $L=1\text{nm}$ . In this figure the miniband formation for energies below the barrier energy maximum is clearly observed for  $H$  below 0.5nm. The width of the minibands considerably increases when the spacing is reduced below 0.5 nm. Fig. 5(b) plots the energy as function of the Si-layer thickness and spacing for  $L=H$ . For very low dimensions, typically below 0.5nm, minibands formation below the barrier energy maximum is clearly obtained (due to wave function overlap when the spacing between quantum wells is low) combined with the strong increase of the meta-material bandgap (due to the 1-D quantum confinement of the energy levels when the Si-layer is very thin). As expected, when the system dimensions increase the minibands evolve to discrete energy levels (as for single quantum wells) and the meta-material bandgap is reduced, reaching the Si-bulk value for  $L=H>6\text{nm}$ .

## 4) Acknowledgements

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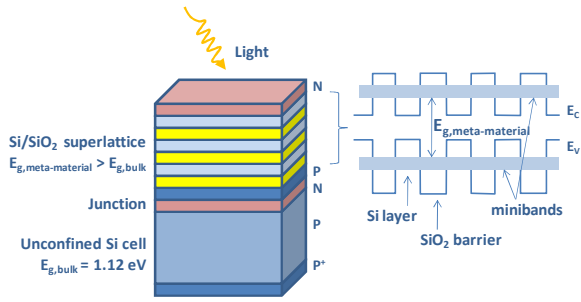


Figure 1. Schematics of a “all silicon” tandem solar cell with a top cell based on a nanostructured meta-material stacked on an unconfined Si cell.

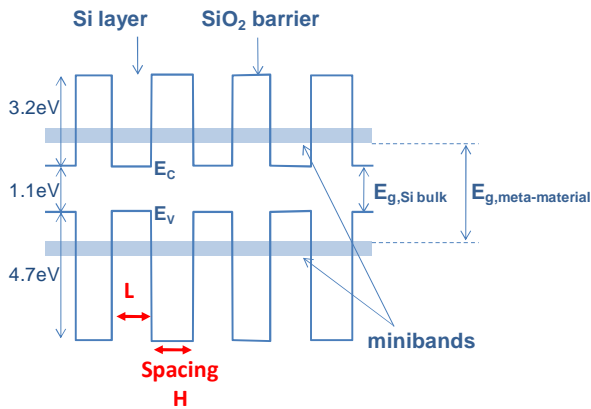


Figure 2. Potential band diagram of the Si/SiO<sub>2</sub> quantum well superlattice and corresponding values of band offsets and bandgaps. The miniband formation below the maximum of the energy barrier is also schematically indicated.

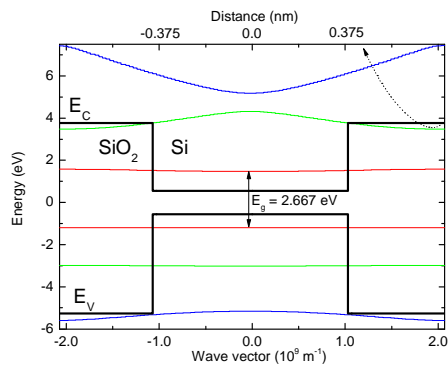


Figure 3. Calculated carrier energy band structure (first three bands) for  $L=H=0.75\text{nm}$ . The meta-material bandgap is also indicated.

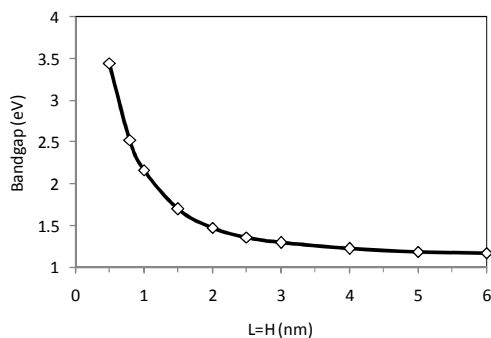


Figure 4. Meta-material bandgap variation with the Si-layer thickness for  $L=H$ .

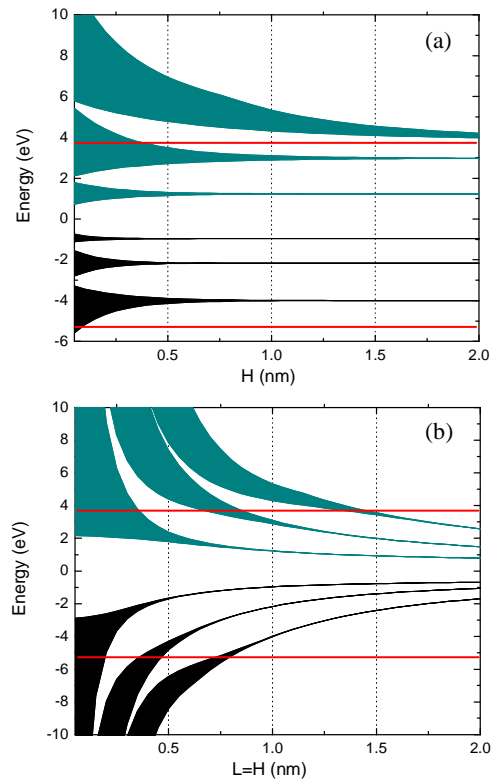


Figure 5. (a) Energy as function of the Si-layer spacing for  $L=1\text{ nm}$  (both conduction and valence band are considered, only the first three bands are shown), showing the minibands formation for energies below the maximum barrier energy for  $H<0.5\text{ nm}$ . (b) Energy as function of the Si-layer spacing and thickness, with  $L=H$ . The maximum of the barrier energy is also indicated for both conduction and valence bands (red lines).

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