

MEASUREMENT OF THE ABSORPTION COEFFICIENT IN SiGe QUANTUM WELLS

Bernd Bitnar, Günther Palfinger, Detlev Grützmacher, Hans Sigg, Stefan Stutz

Paul Scherrer Institut, CH-5232 Villigen PSI
phone: 0041 56 310 4085, fax: 0041 56 310 2646
email: bernd.bitnar@psi.ch, <http://lmn.web.psi.ch/shine/index.html>

This work investigates the use of SiGe nanostructures for photovoltaic devices. In $\text{Si}_{1-x}\text{Ge}_x$ the band gap of the material can be adjusted by changing the Ge content x . This allows an optimal match of a photocell band gap to a given radiation source, which is of crucial interest in thermophotovoltaics [1, 2]. But in solar photovoltaics, as well, the adjustment of a solar cell band gap can increase the efficiency of a single junction photocell. For tandem cells, a SiGe bottom cell allows an optimised current match to the top cell by choosing the best suitable band gap.

SiGe nanostructures can be grown epitaxially onto silicon. Due to a difference in the lattice constant of Ge and Si of 4.2 %, the strained layers have to be thinner than a critical thickness, which depends on the Ge content [3]. This allows the ingrown of SiGe nanostructures in the space charge region of a Si photocell, to shift the band gap to lower photon energies [4].

A highly important question about the utility of SiGe nanostructures for photocell applications is the absorption coefficient in this material system. The absorption coefficient depends on:

- *Ge content x and layer thickness*, which is limited by the critical thickness [3]: In multilayer structures, the average Ge content determines the critical thickness of the layer stack. Growing multilayer stacks with thick Si spacers allows the deposition of more SiGe material compared to a single layer.
- *Strain*: Strain decreases the band gap of SiGe material [5] and should therefore enhance the absorption coefficient compared to unstrained material with the same Ge content x .
- *Confinement shift* of energy levels in quantum structures: The fundamental band gap in a given SiGe material is increased in thin quantum wells [6].
- *Spatial localisation* of charge carriers in quantum structures: It is assumed that localisation enhances the absorption coefficient in nanostructures compared to the corresponding bulk material.

For the measurement of the absorption coefficient in SiGe nanostructures, SiGe multilayer structures were grown on both sides of a Si wafer in an UHV-CVD batch reactor. The deposition parameters are described in [6]. TEM micrographs of our SiGe samples are shown in [6, 7]. An overview of the processed samples is given in the following table, in which n means the number of layers, d_{SiGe} the thickness of each single layer, x the Ge content and $d_{\text{tot}}=n \cdot d_{\text{SiGe}}$ the total thickness of SiGe material:

n	d_{SiGe} [nm]	x	d_{tot} [nm]
30	3.3	0.3	100
10	5.4	0.45	54
20	3.4	0.45	68
40	2.5	0.45	100

To determine the expected weak absorption signal, an internal multiple reflection geometry was chosen, which allows a 400 x light penetration through the layer stack. The measurement setup as well as the evaluation of the absorption coefficient in the layers from the measurement is described in detail in [6].

The result of our measurements is shown in Fig. 1. The absorption coefficient of the 4 SiGe samples compared to absorption data of SiGe bulk material from [8] are shown together with the measurement of a pure Si reference and Si absorption data from [9]. Due to the measurement method, the absorption coefficient could be determined only at photon energies below 1.05 eV and the Si absorption below 1.07 eV.

The following results can be obtained from Fig. 1:

- The SiGe structures show a strong enhanced absorption compared to pure Si.
- The absorption coefficient increases with increasing Ge content.
- For the samples with $x=0.45$, the absorption coefficient decreases with decreasing layer thickness, because in thinner samples the fundamental band gap increases due to quantum confinement.
- Strain, on the other hand, decreases the fundamental band gap compared to bulk material. The sample with $x = 0.45$ and $d_{\text{SiGe}} = 5.4$ nm shows a higher absorption coefficient for $E < 0.95$ eV than bulk material with $x = 0.75$. Considering strain as well as quantum confinement, in [6] fundamental band gaps for the

samples with $x = 0.45$ of 690 meV (for $d_{\text{SiGe}} = 5.4$ nm), 720 meV for (for $d_{\text{SiGe}} = 3.4$ nm) and 750 meV (for $d_{\text{SiGe}} = 2.5$ nm) were calculated.

- A detailed analysis given in [6], in which the absorption coefficient of the quantum well samples is compared with bulk SiGe with a corresponding band gap, does not show any hint of enhancement of the absorption coefficient due to spatial localisation of the charge carriers in thin quantum structures.

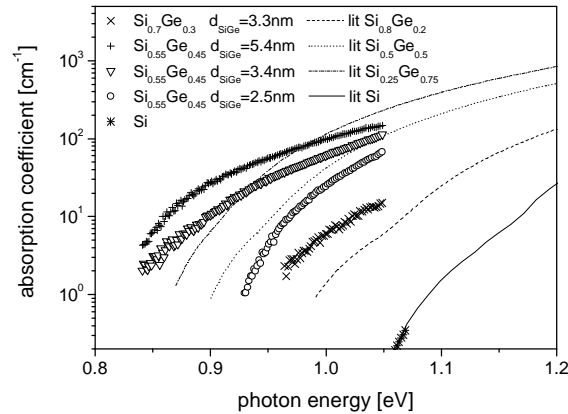


Fig. 1: Absorption coefficient of 4 different SiGe nanostructures compared to pure Si and bulk SiGe from [8].

For a useful application of SiGe nanostructures in photocells a minimum absorption coefficient can be estimated. Assuming a total thickness of the structure in the order of 100 nm because of the limited critical thickness and a light trapping factor of 10 gives an effective absorption length of about 1 μm . Requiring an absorption of at least 10 % at a given photon energy results in an absorption coefficient of at least 10^3 cm^{-1} . From Fig. 1 it can be seen that the absorption coefficient of our SiGe nanostructures below the Si band gap is at least one order of magnitude too low for photocell applications.

An improvement in absorption possibly can be achieved with Ge quantum dots, which contain a higher Ge content than our structures and spatially localise the carriers in 3 dimensions. The Ge quantum dot photocell described in [4] suffers from a too weak increase in short circuit current to overcompensate the loss in open circuit voltage compared to a Si reference.

In conclusion, more experiments are necessary to judge, if SiGe nanostructures will be able to match the band gap and increase the efficiency of Si photocells.

References

- [1] B. Bitnar, W. Durisch, J.-C. Mayor, H. Sigg, H.R. Tschudi, "Characterisation of rare earth selective emitters for thermophotovoltaic applications", *Solar Energy Mat. and Solar Cells* **73/3** (2002), pp. 221 - 234.
- [2] B. Bitnar, J.-C. Mayor, W. Durisch, A. Meyer, G. Palfinger, F. von Roth, H. Sigg, "Record electricity-to-gas power efficiency of a silicon solar cell based TPV system", *Thermophotovoltaic Generation of Electricity: Fifth Conf. on Thermophotovoltaic Gen. of Electr. (AIP Conf. Proc. 653) ed Coutts, Guazzoni, Luther* (2003), pp. 18 - 28.
- [3] R. People, J.C. Bean, "Calculation of critical layer thickness versus lattice mismatch for $\text{Ge}_x\text{Si}_{1-x}/\text{Si}$ strained-layer heterostructures", *Appl. Phys. Lett.* **47** (3), pp. 322 – 324 and *Appl. Phys. Lett.* **49** (4) ,p. 229.
- [4] J. Konle, H.Presting, H. Kibbel, "Self-assembled Ge-islands for photovoltaic applications", *Physica E*, at press.
- [5] C. G. Van de Walle, "Band lineups and deformation potentials in the model-solid theory", *Phys. Rev. B* **39** (3) 1989, pp. 1871 – 1883.
- [6] G. Palfinger, B. Bitnar, H. Sigg, E. Müller, S. Stutz, D. Grützmacher, "Absorption measurement of strained SiGe nanostructures deposited by UHV-CVD", *Physica E*, in print.
- [7] B. Bitnar, G. Palfinger, W. Durisch, J.-C. Mayor, D. Grützmacher, H. Sigg, J. Gobrecht, "Simulation- and demonstration model of a high efficiency thermophotovoltaic system", *Proc. 14th Quantsol Workshop 2002*, editors: DeCola/Königstein/Vanmaekelbergh, pp. 69 - 70.
- [8] E. D. Palik, *Handbook of Optical Constants of Solids Vol. II*, Academic Press 1991, pp. 607 – 636.
- [9] M. A. Green, M. J. Keevers, "Short Communication: Optical Properties of Intrinsic Silicon at 300K", *Progress in Photovoltaics: Research and Appl.* **3** 1995, p. 189.