**Research related part**

A significant increase in energy consumption and reduction of conventional fossil fuels in the world causes increased attractiveness of renewable energy sources. The European Council has set a goal to reach 20% of renewable energy in the total energy consumption in the EU by 2020. Among the renewable energy sources the sun is the most promising, because it is free and endless for any user. The main goal for the researchers is to increase the photovoltaic conversion efficiency and to decrease the price per watt and the price of the produced kilowatt-hour. At the same time, a requirement of large-scale production leads to limitations in the choice of materials used for solar cells fabrication. It should be abundant and environmentally friendly (not toxic). Striking examples of highly efficient solar cells, which do not satisfy these conditions, are CuInGaSe (CIGS) cells. According the “U.S. Department of Energy” studies, the natural source of indium and gallium is extremely limited [G. Kavlak et al., 40th IEEE, 1442 (2014)]. CdTe solar cells use the rare metal tellurium and the toxic metal cadmium and therefore specific requirements for the recycling of these panels should be applied. From this point-of-view silicon-based solar cells are of the greatest interest. The world stock of silicon is unlimited and technology of manufacturing, cleaning and processing is well developed. From today's perspective, the third generation of solar cells will be realized on the basis of nanomaterials. There is a statement from two well-known experts in this field, Dr. Joris Libal and Dr. Radovan Kopecek, they suggest that there will be no replacement of G1 PV modules in the near and mid-term future – rather a slow transformation to G3 PV modules by using advanced c-Si technology in combinations with various nanotechnologies at a cell and module level [18] Solar cells based on silicon take almost 95% of the total terrestrial photovoltaics. Normally silicon-based solar cells are divided into two main groups:

thin film solar cells based on amorphous hydrogenated (a-Si:H) and microcrystalline (µc-Si) or nanocrystalline (nc-Si) silicon, fabricated at relatively low temperatures (<300°C) on glass or flexible substrates. The advantage of such cells is the cost-effective low temperature large area thin film technology. The drawback of such solar cells is low efficiency, usually not exceeding 10% [1-3].

solar cells based on mono - and polycrystalline silicon wafers have higher efficiency (at average 16-20% in production). However, the fabrication process of such devices requires high temperatures, which causes them to be rather expensive and imposes a limitation on the minimum thickness of the substrate.

Photovoltaic (PV) modules can potentially be produced much cheaper than today when moving from bulk wafer cells to thin film cells on cheap substrates such as flexible polymer. Thin film modules are made by integrating a several micrometer thin active device layer on cheap supporting substrates like foils of metal or polymer. Best prognosis to dominate the PV market in the long run is given for thin film non-toxic, abundant and durable silicon. Right now exploitation of thin film silicon PV is not carried out to its full extent due to a lack of high efficiencies and good reliability of today’s silicon thin film solar cells. The silicon-based approaches are certainly favoured because of material abundance and non-toxicity at a high level of materials control and understanding together with a huge industrial infrastructure to account for low production/processing costs and high production yields. The next promising path for photovoltaic development is the usage of silicon nanowires (SiNWs) [4-7]. Silicon nanowires allow a variety of advantages - from enhanced light trapping to quantum size effects - like variation of the band gap and enhanced direct band absorption [8-10]. The last opens a new way for full silicon multi-junction solar cell development, where a top junction is based on silicon nanowires and the bottom junction is based on mono-crystalline silicon. Recently, promising results were obtained on single-nanowire silicon solar cells and microwire arrays [7, 11-13]. An excellent passivation of the silicon surface by a-Si:H films was demonstrated by successful development of a-Si:H/c-Si heterojunction solar cells [14-17].

1. Here is a part related to the thermal transport inn solar cell: problem description, monitoring and possible problem controlling solutions
2. The part related to the photovoltaics industry current level and perspectives in Ukraine should be discussed.

Our proposal correlates exactly with the idea of Libal & Kopecek about transformation of G1 solar cells into the 3G solar devices. The main aim of the proposed project is a fundamental focus to the novel solar cell device based on 3D structured silicon realized on flexible substrates. The proposed design of 3D solar cells is shown in *Fig. 1*. A flexible substrate with back contact layer is covered by a crystallized silicon film, which has multi-crystalline structure. The BSF (back surface field) layer is formed on the back side of the multi-crystalline silicon (mc-Si), while the front surface has a vertically-aligned architecture. Silicon wires of submicron diameters and micron length are formed by etching. A wide band gap emitter layer (doped a-Si:H or GaP film) deposited at low temperature on the top surface of the mc-Si forms an isotype heterojunction being the bottom junction of the multi-junction solar cell. Further, heavily doped a-Si:H or µc-Si layers are deposited to form a tunnel junction for electrical connection between the top and bottom photoactive junctions. An intermediate transparent conductive oxide layer (TCO) for better optical confinement is also considered. A top p-i-n a-Si:H junction is deposited on the columnar surface. Finally, a TCO layer covers the surface of the solar cell for top contact, which will be connected via a metal grid.

|  |  |
| --- | --- |
| Dfg flex 2  a) | rect850  b) |

**Figure 1**: Schematically cross-section view of a 3D multi-junction solar cell based on nanostructured silicon realized on a flexible polymer (a) and a metal foil (b).

By the end of the proposed project we are expecting to achieve the following results:

* To clarify the influence of the silicon nanostructures dimension (diameter, length, density) to the PV performance in correlation to theoretical and experimental studies in such hetero-junction layer stacks;
* To theoretically and practically evaluate the influence of the heterojunction interface surfaces to the electrical transport and recombination processes;
* To investigate the physical characteristics of PV-device and specific electrical transport mechanism
* To investigate the thermal processes and possible controlling mechanisms

The main goal of the “XXX” project is to find theoretical and practical bases for development of high efficiency solar cells using 3D silicon nanostructures. It is a complex task, which requires an interdisciplinary consortium capable of addressing all relevant issues from nanoparticle template formation, 1D semiconductor nanostructures formation, analysis of physical properties and device fabrication. In this proposal we suggest therefore a transnational cooperation between the Leibniz Institute of Photonic Technology (IPHT) , France, Ukraine, where partners have a significant experience in the field of the proposed subject.

There are lots of technological and physical fundamental problems to be studied in the framework of the project including different aspects of PV materials and devices development:

• study of the electrical properties of the 3D silicon nanostructures including specific transport mechanisms;

• study of the surfaces and hetero-interfaces properties of the silicon 3D nanostructures and their influence to electrical transport and recombination phenomena;

• study of materials interaction in nano-size scale during silicon nanostructure fabrication;

• physical and chemical aspects of silicon wires surface modification in plasma;

• study of the structural and optical properties of the 3D silicon nanostructures;

• control the size and density of silicon wires;

• surface passivation technology development;

• 3D device design development using computer simulations.

* Thermal effects, transport etcc.

In order to provide a clear structure of the work plan, four work packages have been defined:

**WP1 Formation and characterization of microcrystalline silicon layers on flexible surfaces.**

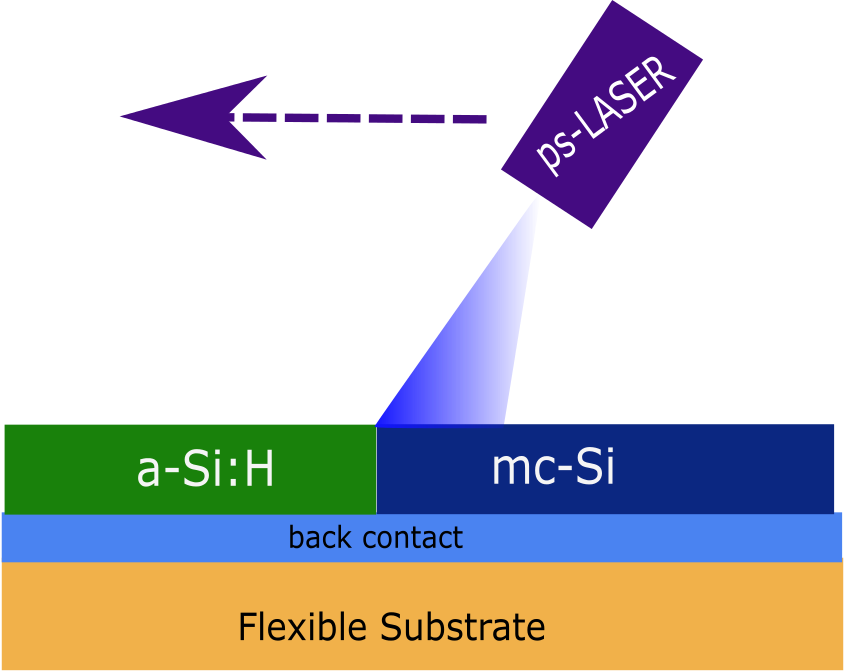
(i) formation of microcrystalline silicon layers on flexible substrates (polymer and/or metal foil) using low temperature processes like PECVD and evaporation technique; for the crystallization of amorphous silicon layers the solid phase or laser induced crystallization will be applied (IPHT);

(ii) formation of silicon nanostructures using wet-chemical (IPHT)) approaches;

(iii) evaluation of the microstructure and topology will be performed using a combination of focused ion beam (XXXX), Raman spectroscopy (XXX) and electron backscatter diffraction (EBSD; XXX).

For the realization of the proposed soar cell architecture, several major technological steps will be developed and optimized.

The first main step is the laser crystallization of amorphous silicon. Amorphous silicon will be evaporated or sputtered onto silicon wafers (firstly) and flexible substrates: metal or polymer foil. Next, the amorphous silicon will be crystallized using a ps-laser as shown in Fig. 1. The IPHT has a wide experience in silicon laser crystallization and solid phase crystallization of amorphous silicon [7, 19].



**Figure 2: Schematically representation of the laser crystallization of a-Si layer.**

Silicon nanowires will be formed by wet etching. Two main etching techniques will be involved namely: wet chemical and dry plasma etching. The wet chemical etching technology using Ag catalysis is well developed at the IPHT [20]. Vertical and zig-zag inclined nanowires could be successfully obtained as shown in Fig. 3. An advantage of this technique is, that no radiation defects are created during the etching.



**Figure 3: Scanning electron microscopy micrographs of vertical (left) and 45° zig-zag (right) silicon nanowires obtained by wet etching at the IPHT (Jena/Germany).**

The microstructure and topology of the surface will be investigated using electron microscopy and diffraction methods (XRD, EBSD).

**WP2 Formation and characterization of cover layers around 1D silicon structures.**

(i) formation of wide band gap emitters: a-Si:H using PECVD and GaP using coupling of PECVD-ALD (XXX);

(ii) formation of tunnel and p-i-n junctions using PECVD ((XXX);) and sputtering (XXX); techniques;

(iii) formation of a TCO layer using ALD/MOCVD ((XXX);) and sputtering (XXX);) techniques;

(iv) microstructure and topology characterization of each layer stack in the 3D device using SEM, FIB, Raman, EBSD, XRD, TEM, PL, reflectance and absorption studies ((XXX);).

The vertically-aligned design of top p-i-n junctions is a way to enhance absorption in undoped a-Si:H intrinsic layers without rising (or ever with reducing) its thickness and therefore it allows one to increase short circuit current (Jsc). For multi-junction solar cells, the Jsc generated by each sub-cell should be equal because of serial connection of the sub-cells. It is the so called current matching condition. From this point of view there is an optimum value of band gaps for multi-junction solar cells. In case of a bottom silicon junction, a gap for a top junction should be in the range of 1.6...1.8 eV and a Si:H suit this condition well. In order to reach an optimum short circuit current level (Jsc approximately 20 mA/cm2), the thickness of a Si:H should be of few microns for better absorption. Unfortunately, when the thickness of the i-layer in p-i-n junctions exceed a critical value (200-300 nm in case of a-Si:H) an electric field decreases, leading to increasing recombination losses and a drop of the open circuit voltage (Voc) and as consequence to a loss of efficiency. In this way a classic planar approach to a-Si:H/c-Si tandem solar cells cannot be realized. However, in the proposed design one can increase Jsc due to vertical allocation of a-Si:H i-layers deposited on the well of the silicon wires and additional optical confinement of the wired surface. In this case we can achieve an increase of effective thickness, while no reduction of Voc is expected, because the physical thickness and therefore the electric field remain the same. The way to reduce the thickness of an undoped a-Si:H layer in p-i-n junctions will be also considered. If we can keep the Jsc value with reduction of the i-layer thickness, the efficiency of the top junction should be higher while the light induced degradation effect becomes weaker. Concerning the bottom junction, the quality of crystallized silicon, which is determined mostly by the lifetime of minority carriers, is far from that of monocrystalline wafers. Nevertheless, solar cells of 8-10 % efficiency were obtained with laser crystallized silicon/a-Si:H heterojunctions at IPHT. Thus the combination of high efficiency 3D p-i-n a-Si:H solar cells with a Si:H/mc-Si heterojunctions on flexible light substrate should allow us to reach approximately 15-17 % level of efficiency, being at the average level of bulk Si crystalline cells and considerably higher as compared to conventional a-Si:H/µc-Si thin film tandem solar cells. Development of this new way in photovoltaics is a goal of this project.

There are two approaches to back contact and BSF layer formation. The first one means point metal contacts at the back side of the polymer foil fired by a ps-laser. The second one is based on diffusion of Al from a multilayer contact film during silicon crystallization. The Al layer being a source of III-atoms (acceptors for silicon) is covered by a thin diffusion barrier layer (Cr or W). A diffusion barrier is required to limit Al diffusion into Si to only local area near to the back surface.

An amorphous hydrogenated silicon shell layer will be deposited by PECVD. This is a common used technique for high quality a-Si:H film deposition, which allows one to cover the whole surface of Si nanowires as demonstrated in Fig. 4a. Another approach to the bottom heterojunction will also be explored in the project. The low temperature (less than 400°C) plasma-enhanced atomic layer deposition (PE-ALD) of a GaP layer developed in SPbAU will be used to form the wide gap emitter to mc-Si. This technique is based on an alternating change of the phosphorus and gallium atom source flows, providing the growth of one monolayer by cycle. It allows one to obtain atomically smooth 2D-surfaces without island 3D-growth (Fig. 4b). Thin epitaxial GaP layers, grown at low temperature and lattice-matched to silicon, could provide good passivation of the GaP/Si interface, which is required for high efficiency Si based solar cells.

Transparent conductive oxide (TCO) deposition will be realized using magnetron sputtering ((XXX) and atomic layer deposition (ALD at IPHT) techniques. ALD is a modified chemical vapor deposition (CVD) technique and offers the possibility to deposit monolayer (ML) scale films of high uniformity, particularly on high aspect ratio structured surfaces. Different conducting, semiconducting and a large number of dielectric materials can be deposited by ALD. Zinc oxide (ZnO) as well as aluminium doped zinc oxide (Al:ZnO or AZO) can also be deposited with high conductivity and high optical transmission by this technique and thus applied as TCO materials. The benefits in using Al:ZnO instead of ITO in ALD are lower costs, the more simple precursor chemistry and thus the easier realization of the ALD process. The marginal deficit in conductivity of Al:ZnO compared to that of ITO is negligible in this case. Thus ALD is very suitable for producing multi-junction solar cells with 3D architecture. The different type of TCO films such ITO, ZnO:Al and/or SnO2:F will be explored.

|  |  |
| --- | --- |
| **a)** | **b)** |

Figure 4: SEM cross-sectional view of silicon rods covered by an a-Si:H layer using PECVD (a) and a GaP layer deposited on Si by low temperature PECVD-ALD (b) at SPbAU.

**WP3 Evaluation of 3D multi-junction PV device based on 1D silicon.**

(i) simulation of a 3D multi-junction layers stack ((XXX);

(ii) formation of a 3D device using monocrystalline and polycrystalline (PV) silicon single wafers (XXX, IPHT);

(iii) evaluation of the I-V, C-V and optoelectronic 3D device properties ((XXX, IPHT);

(iv) transfer of a 3D layers stack on structured microcrystalline silicon to flexible surfaces (XXX, IPHT).

For analytical expressions of the optical and electrical properties (absorption, work function, I-V characteristics, quantum efficiency, etc.) of the layer/s stack/s, the theoretical modeling using AFORS-HET and Silvaco ATLAS software (developed for the simulation of multi-layer semiconductor heterostructures) will be carried out. Silvaco ATLAS software allows us to simulate 2D and 3D structures, which is very important with regard to the project tasks. Simulation programs perform a numerical solution of the continuity and Poisson's equations for each layer using different boundary conditions and external influences (applied voltage, lighting). Hetero-interface parameters can be specified by introducing a very thin (a few nanometers) surface layer between the two semiconductor layers. The band diagram, main solar cell characteristics and various electrical measurements can be simulated, which allows one to forecast the experimental results. Simulations may sufficiently predict the properties of heterostructures of different design, when real parameters of the layers and interfaces obtained from the previously mentioned characterization techniques are introduced. Theoretical simulations allow us to get recommendations for multi-junction design optimization.

The uniformity and microstructure of the grown layers and fabricated structures will be characterized by scanning electron microscopy (SEM), transmission electron microscopy (TEM), electron backscattered diffraction (EBSD), atomic force microscopy (AFM) and Raman spectroscopy. Optical properties are investigated by photoluminescence (PL) measurements, including mapping for heterogeneity studies.

Regarding the electrical properties, special attention will be paid on the study of heterojunction interfaces, electronic properties of the a-Si:H and mc-Si layers volume properties. The main experimental studies of the grown structures will be performed by PL, quasi steady state photoconductivity (QSSPC), admittance spectroscopy, deep level transient spectroscopy, capacitance-voltage profiling, current-voltage characteristics and spectral response measurements.

**WP4 Acoustics and thermal processes……**

**References:**

1. K. Lips, P. Kanschat, W. Fuhs, Sol. Ener. Mater.&Sol. Cells 78, 513 (2003)

2. S. Gall, J. Schneider, J. Klein, K. Hübener, M. Muske, B. Rau, E. Conrad, I. Sieber, K. Petter, K. Lips, M. Stöger-Pollach, P. Schattschneider, W. Fuhsa, Thin Solid Films 511–512, 7 (2006)

3. J. Haschke, L. Jogschies, D. Amkreutz, L. Korte, B. Rech, Sol. Ener. Mater.&Sol. Cells 115, 7 (2013)

4. V. Sivakov, F. Voigt, B. Hoffmann, V. Gerliz, S. Christiansen, Wet- Chemically Etched Silicon Nanowire Architectures: Formation and Properties. Intech; "Nanowires - Fundamental Research", ISBN 978-953-307-327-9; ed. Abbass Hashim; Chapter 3, 45-80 (2011)

5. A.I. Hochbaum, R. Fan, R. He, P. Yang, Nano Letters 5, 457 (2005)

6. B.A. Buchine, F. Modawar, M.R. Black, US Patent US8143143 B2 (2012)

7. V. Sivakov, G. Andrä, A. Gawlik, A.Berger, J. Plentz, F. Falk, S. H. Christiansen, Nano Letters 9, 1549 (2009)

8. B.M. Kayes, N.S. Lewis, H.A. Atwater, J. Appl. Phys. 97, 114302 (2005)

9. V. Sivakov, F. Voigt, G. Bauer, S. H. Christiansen, Phys. Rev. B 82, 125446 (2010)

10. S.Misra, L. Yu, M. Foldyna, P. Roca i Cabarrocas, IEEE Journal of Photovoltaics 5, 40–45 (2015)

11. M.D. Kelzenberg, D.B. Turner-Evans, B. M. Kayes, M. A. Filler, M. C. Putnam, N. S. Lewis,

and H. A. Atwater, Nano Letters 8, 710 (2008)

12. M.C. Putnam, S.W. Boettcher, M.D. Kelzenberg, D. B.Turner-Evans, J.M. Spurgeon,

E.L. Warren, R.M. Briggs, N.S. Lewis and H.A. Atwater, Energy Environ. Sci. 3, 1037 (2010)

13. M. Al-Ghzaiwat, M. Foldyna, T. Fuyuki, W. Chen, E. V. Johnson, J. Meot, P. Roca i Cabarrocas, Scientific Reports 8, 1651 (2018)

14. T. Mueller, S. Schwertheim, and W.R. Fahrner, J. Appl. Phys. 107, 014504 (2010)

15. N. Jensen, U. Rau, R.M. Hausner, S. Uppal, L. Oberbeck, R.B. Bergmann und J.H. Werner, J. Appl. Phys. 87, 2639 (2000)

16. A. Froitzheim, K. Brendel, L. Elstner, W. Fuhs, and M. Schmidt, J. Non-Cryst. Solids 299-302. 663 (2002)

17. M. Schmidt, L. Korte, A. Laades, R. Stangl, Ch. Schubert, H. Angermann, E. Conrad, Thin Solid Films 515, 7475 (2007)

18. J. Libal, R. Kopecek, ISC Konstanz. Limit for industrial c-Si solar cells reached in 2030: http://www.pv-tech.org/guest blog/limit\_for\_industrial\_c\_si\_solar\_cells\_reached\_in\_2030\_what\_next

19. F. Falk, G. Andrä, EU Patent EP1,314,208 B1, May 28th (2003); (42) F. Falk, G. Andrä. U.S. Patent 7,091,411 B2, Aug. 15th (2006).

20. V. Sivakov, G. Brönstrup, B. Pecz, A. Berger, M. Krause, G. Z. Radnoczi, S. H. Christiansen,

J. Phys. Chem. C 114, 3798–3803 (2010).

**BUDGET Planning**

***By total project budget of 1.500.000 €***

***For Scientific Part (research): 30% or 450.000€***

*UKR: 70% or 315.000€*

*FR+GER: 30% or 135.000€*

***For Dissemination Part (research): 70% or 1.050.000€***

**IPHT (needs)**

**Research activities: approx. 450T€**

*Scientific Staff* at Leibniz IPHT (36MM); 1 Engineer (18MM); 1 PostDoc (36MM): 350.000€/3Y

Consumables: Wafers (5T€), ALD Precursors (10T€); Chemical filters (10T€); CVD Precursors (5T€); Chemicals for etching (10T€); Laser crystallization (5T€); CVD and EBE targets, Knudsen cells (10T€): 55.000€/3Y

Conferences: 21.000€/3Y

Visits to Ukraine: 3 times per year. Duration 14 days. 21.000€/3Y

Visits to France: 2 times per year Duration 7 days. 9.000€/3Y

**Dissemination activities**: **approx.. 80T€**

Workshop in UKR with UKR PV industry (as example): participation (2 Persons)

Workshop in UKR with regional PV industry (2 Persons)

Meeting with UKR government:

Summer school in UKR related to the PV and material science (5 Persons)

Workshop in Germany for early carrier stage students from UKR, GER and FR (organization)

Workshop in Germany for young leaders from UKR, GER and FR (organization)

Annual meetings in UKR and FR: 2 times per year. Duration 2 days. 6.000€/3Y

IT licenses: for online platforms

Management: project administration, local workshops and meetings organization, etc.

Annual meetings in GER: 1 time per year. Room, catering, logistics

**UKR**:

**Research activities:**

Research personnel

Research related consumables

Research related small equipment

Research related conferences

Research related staff exchange to GER

Research related staff exchange to FR

**Dissemination activities**:

Internet page: platform and web design

IT licenses: for online meetings

Project management: meetings, workshops, conferences

Project coordination: reporting and monitoring

PV Market research: the PV perspectives in Ukraine: production and installation of solar plants

Workshops with local PV industry (as example) in UKR

Workshop with regional PV industry in UKR

Summer school related to the PV and material science in UKR

Workshop (3 times) in Germany for early carrier stage students from UKR, GER and FR (administration and organization)

Workshop (3 times) in Germany for young leaders from UKR, GER and FR (administration)

Workshop (3 times) for administrative stuff with National (GER and FR) coordination offices and EU project managers from expert institutions (IPHT and Université de Lorraine; expertise and daily experience by working with EU projects organization and management))

Scientific and administrative short-term visits upto 7 days (efficient organization of administrative work at different level in German research institute and French University)

Meeting with UKR government (incl. representants from FR and GER): legal basis for “PV industry in Ukraine: Presence, perspectives and Challenges”

Publicity: TV, press, online promotion

Etc…………

**FR (similar to German one or….)**

………………………..