Digitalization meets PV production technology – Outline of a smart production of silicon solar cells and modules

Martin Zimmer, Matthias Demant, Norbert Bergmann, Stefan Rein, Jochen Rentsch & Ralf Preu,
Fraunhofer ISE, Freiburg, Germany.

Abstract

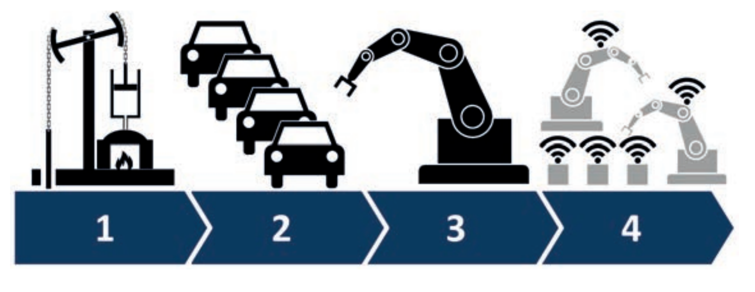
Ever since the manufacturing of PV modules began suffering from a huge price decline, the reduction of the production cost has been a task of high priority. Digitalization is a subsequent further development of the automation of today's PV cell and module manufacturing processes and can help to decrease production costs. A central concept of digitalization is the *digital twin*, which represents the properties and behaviours of physical assets, materials, processes or eventually the entire production line (the so-called *smart fab*). Different cases of its use are presented in this paper, along with a discussion of the corresponding applications of such digital twins. Finally, a smart fab for PV production is described.

Introduction

Digitalization has been an ongoing process for over two hundred years, reducing production costs in many industries. The development of digital manufacturing goes back to the beginning of the 19th century, when the first digital production tools were invented, allowing a fast and cost-effective production combined with a high-quality standard. One of the first digital production tools was the *Jacquard loom*, where the pattern of a loomed tissue was stored on punched cards. Today, four industrial ages can be distinguished, which were ushered in by industrial revolutions (Fig. 1).

"Digitalization is now regarded as the next promising strategy for achieving further reductions in production costs."

Figure 1. Schematic of the four industrial revolutions.



Source: https://commons.wikimedia.org/wiki/File:Industry_4.0_NoText.png.

The first industrial revolution was the introduction of mass production, together with the use of steam engines as an energy source; this first industrial revolution can be dated to the late 18th century. The second industrial revolution is characterized by the division of labour and assembly-line production; this started at the beginning of the 20th century, with the most famous example being the switch to a moving assembly line system in 1913 for the production of Henry Ford's Model T. The introduction of computer technology in industrial production in the 1970s is considered to be the third industrial revolution. Central tasks were shifted to microcontrollers – the classical machine controls with hardwired relays and contactors were successively replaced by programmable logic controllers. The whole manufacturing process was increasingly managed by different enterprise resource planning (ERP) applications. The fourth, and current, industrial revolution has been proclaimed to be an ongoing process, where a decentralization of the system intelligence is enforced by the price decline in computing and storage capacity, as well as by the availability of very fast communication networks.

The production of PV devices has shown significant cost reduction over the last decade; on the one hand, this leads to the worldwide success of PV power generation, but on the other, it has put many manufacturers under enormous price and innovation pressure. One important factor for the strong decline is represented by the 'economy of scale' of single manufacturing units up to the multi-GW scale, necessitating also a high degree of automation. Digitalization is now regarded as the next promising strategy for achieving further reductions in production costs [1]. But how can the concrete implementation of digital technologies help to reduce production costs and simultaneously increase product quality?

Degree of digitalization of today's PV production

At the beginning of mass production of PV modules, almost the entire logistics were done manually. Process tools with a throughput of approximately 1,000 wafers per hour were fed and unloaded by operators. Increasing labour cost prompted an urgent development of fast and reliable automation solutions.

Today, a high degree of automation is accomplished in most PV manufacturing sites. The cell manufacturing process begins with the inspection and automated loading of wafers into the required process carriers. All the subsequent process equipment is able to unload wafers from carriers, process the wafers and reload the carriers. The logistic units employed are equipped with radio-frequency identification (RFID) tags, which allow the tracking of the process batches along the whole production chain. The information about the processed batches, together with the process data, is collected by a manufacturing execution system (MES), which centrally collects all the relevant data from the tools.

In summary, the actual state of the art in PV production is what is called *industry 3.0,* characterized by mass production in assembly lines, which is highly supported by central software services.

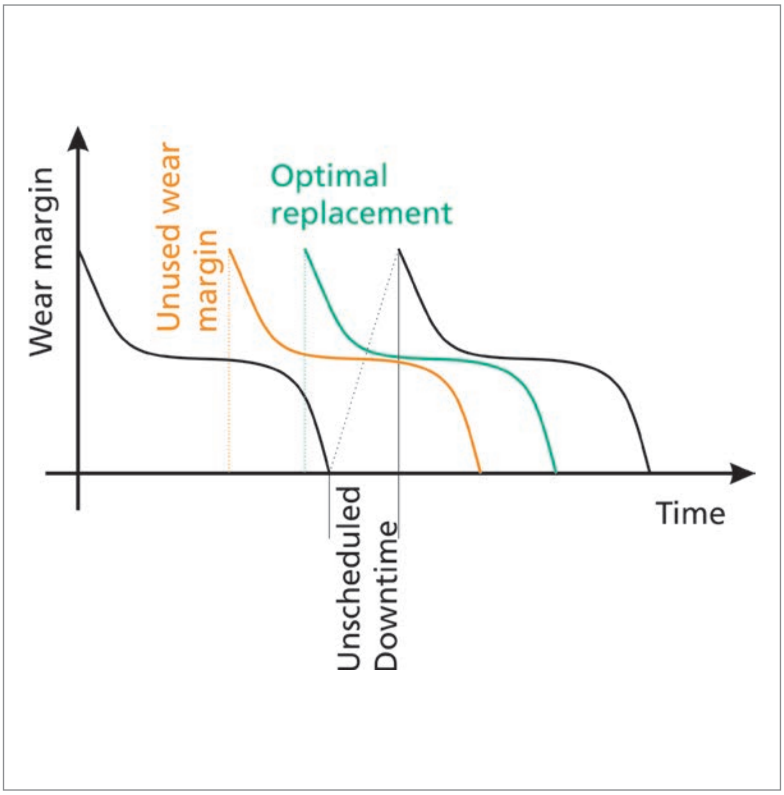


Figure 2. Wear margin usage in different maintenance strategies (black: reactive maintenance; orange: preventive maintenance; green: predictive maintenance).

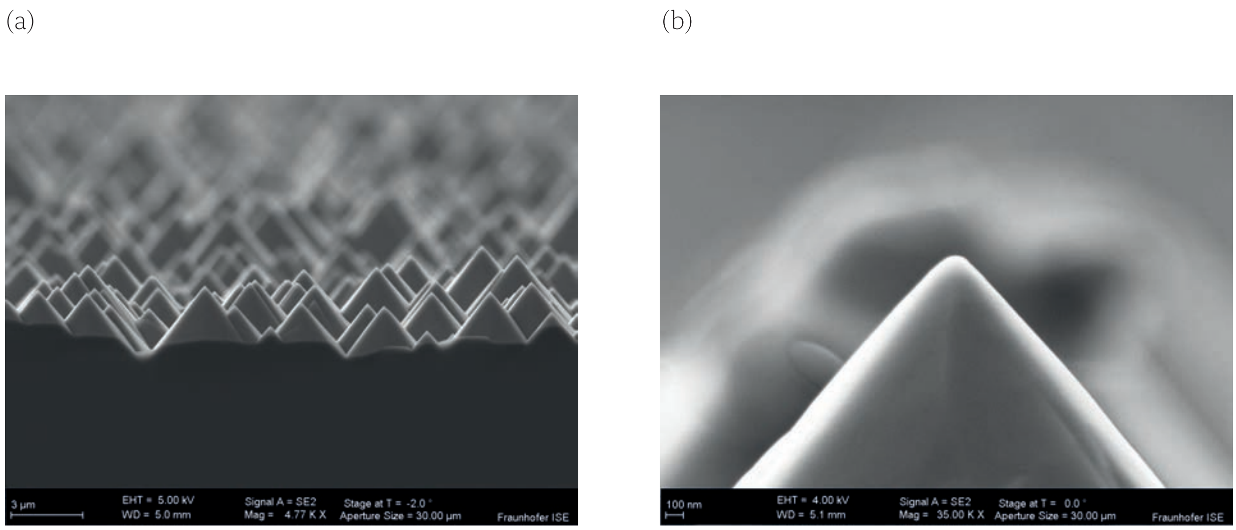


Figure 3. (a) Random pyramids are created in an alkaline etching process on monocrystalline silicon. (b) After an etching in HF/HCl/O3, the pyramid tip is rounded.

A digital future for production

Although the actual production system for PV modules incorporates a central intelligence, which collects, evaluates and reports the entire process and equipment data, a paradigm shift is predicted during the fourth industrial revolution. While equipment data, process data, quality data and metrology data are stored more or less in a single database in common MESs, this business intelligence will be completely distributed over the whole production system.

> "Future process tools will be expected to increasingly work autonomously."

Digital twin concept

In the new paradigm, the intelligence is distributed over several instances, each with a defined task. The concept of a digital twin – also called a *digital shadow* – plays an important role in this. A *digital twin* is a digital representation of a real object which represents the properties and behaviour of this object. A very simple example of a digital twin is a stored ID number, which represents one single instance of a real object; the properties of this object can then be assigned to this ID, so that a digital twin represents the *properties* of this object. A more complex digital twin also represents the *behaviour* of the object. This allows the user to obtain the properties of an object, even if the object is temporarily not connected to the network; moreover, it allows a prediction of the properties of this object in the future. Digital twins of the materials used provide data on the origin and the material properties, while the digital twins of process tools provide all the necessary data for the entire life cycle of the tool. The construction plans from the engineering phase enable the simulation and optimization of the core parts of a tool. Furthermore, this data can be used by virtual reality applications, which facilitate an assisted maintenance: for example, a virtual reality which creates a virtual three-dimensional image of the tool can help in carrying out maintenance tasks.

Digital twin of a process tool

The digital twin of a process tool can provide the geometrical and mechanical data relating to the tool; this enables simulations of the functional properties of the tool to be performed. The digital twin can also contain (or even reference) the digital twins of parts: for example, the digital twin of a wet chemical process tool can contain the digital twins of the circulation pumps used. This can help in the implementation of various useful systems, such as a *predictive maintenance* system.

Predictive maintenance is a maintenance strategy which tries to combine the advantages of preventive maintenance and reactive maintenance [2]. *Reactive maintenance* uses a system until it breaks down, when the wear margin has been

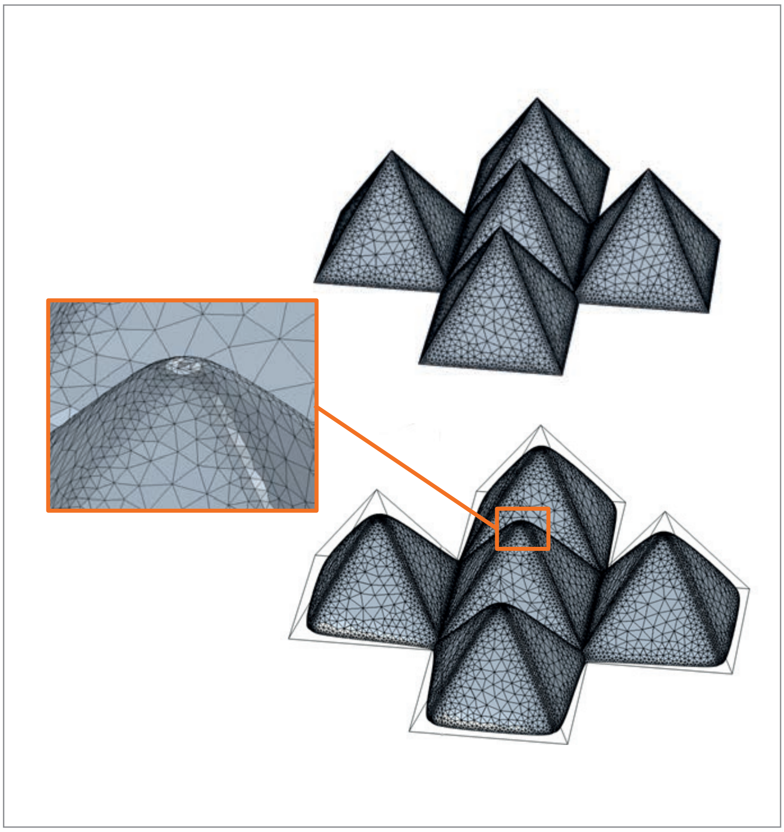


Figure 4. Simulation model for the pyramid rounding in HF/HCl/O_3 (top). Result of the simulated etching on the pyramid tip (bottom).

completely consumed. This strategy makes optimal usage of the wear margin on the one hand, but has to accept unscheduled downtimes of the tool on the other.

In the *preventive maintenance* strategy, consumables are replaced according to a schedule that has been created from empirical values, with no consideration of the individual wear conditions. The resulting avoidance of unscheduled downtimes is achieved by replacing parts with a residual wear margin.

A combination of both the above strategies attempts to find the optimal point for the replacement of each individual component (Fig. 2). This can be done either by direct condition monitoring using sensors, or by evaluating a model which predicts the condition of the components as a function of usage and environmental conditions.

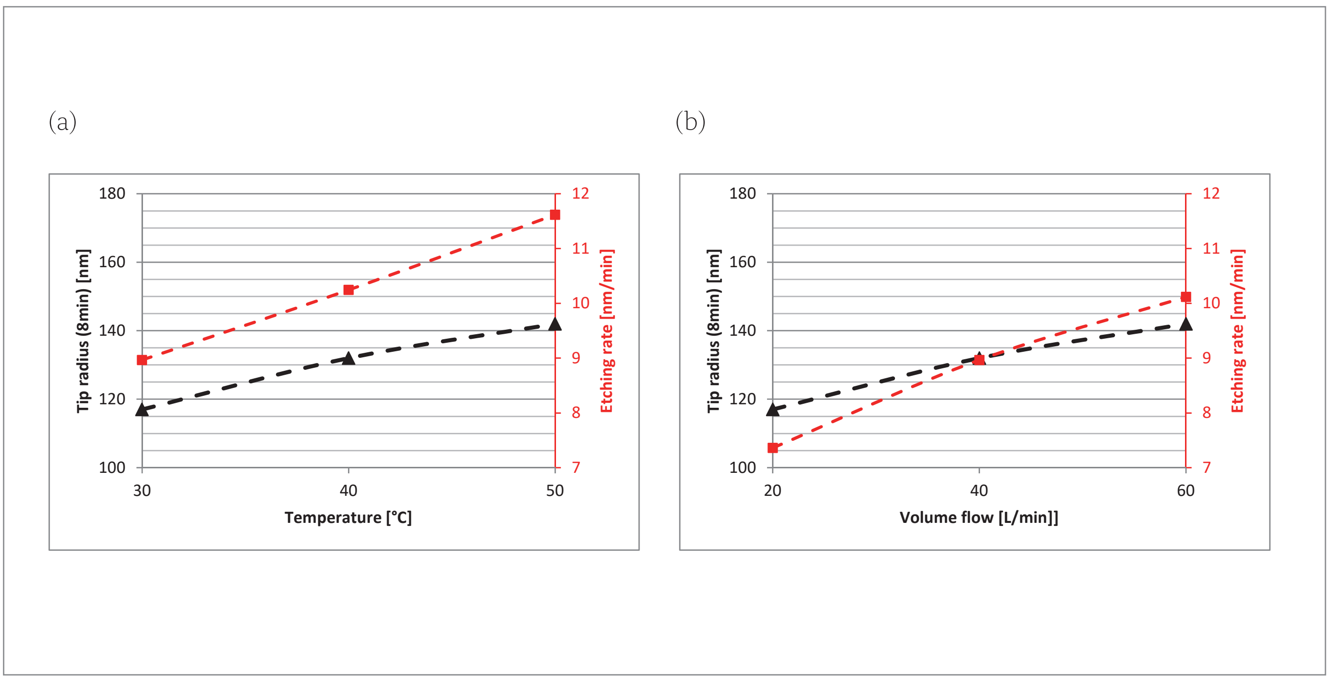
The individual monitoring of components requires additional sensors that enable the prediction of future system breakdowns. An example of such a sensor is ABB's smart sensor [3], which consists of a box that can be mounted on pump motors and contains vibration and temperature sensors. The box monitors the rotational speed of the pump, operating hours, blade problems, looseness, misalignment and pump imbalance, and enables the identification of maintenance requirements.

The implementation of additional sensors can help to monitor the health of critical systems; however, it also runs counter to the need for further reducing cost. Therefore, the implementation of models which predict the wear state by means of usage data (which is accessible via the digital twin) will be an important task in the future, to reduce maintenance costs and unscheduled downtimes.

Modelling of production processes

Digital twins are useful for understanding and optimally using the process equipment. The primary interest, however, is the interaction between the materials used and the equipment. This means that a prediction of process quality has to combine the information from a digital twin of a material with that of a process tool. Meta-models are very important for such an implementation,

Figure 5. Development of the pyramid tip radius and etching rate with respect to (a) temperature, and (b) volume flow.



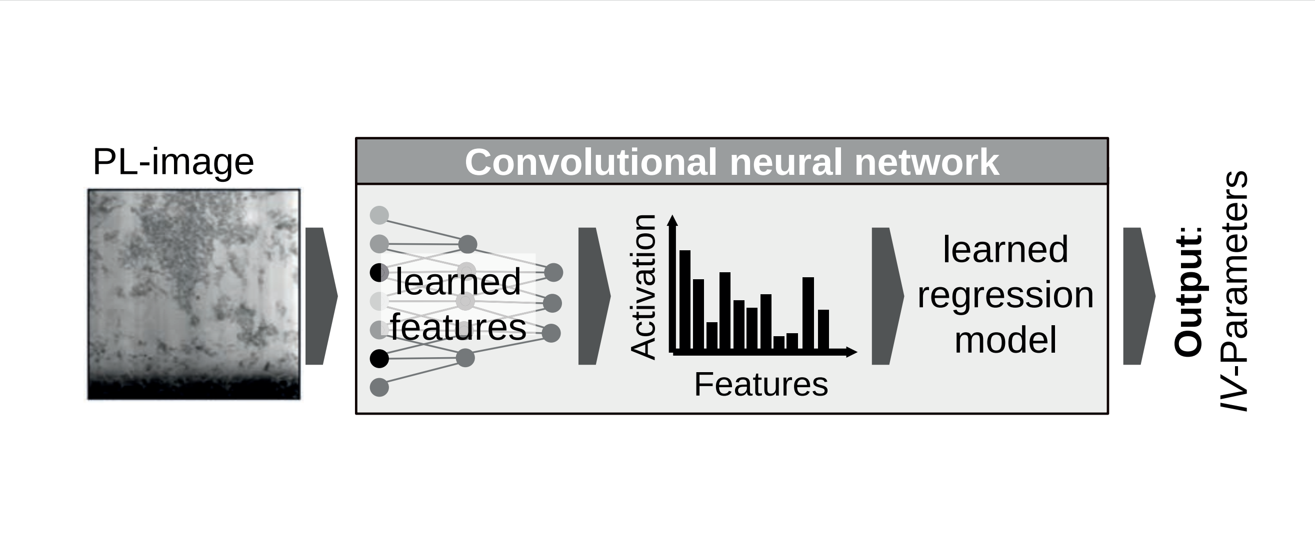


Figure 6. A convolutional neural network directly evaluates PL images of as-cut wafers to predict the solar cell efficiency.

since they allow a correlation between process conditions and process results. The most important parameters in PV production are, of course, the performance data of the final module, as well as the production costs. The implementation of these meta-models is one of the main tasks to take advantage of the digital twins.

Meta-models can use different approaches. In consequence, a digital twin should contain the exact physical parameters of every part of the object. This being the case, fundamental physical equations would predict the state of the object for a defined point in time in the future and a sufficiently well-behaving system. Since this approach is computationally very time intensive, it can only be used in the early stages of the construction of the process tools. For a real-time prediction of production parameters, more advanced semi-empiric and empiric approaches are needed; in this field especially, enormous progress has been made in recent years.

Example of an ab initio process model

Future process tools will be expected to increasingly work autonomously: optimization of the process recipes will be done by the tool itself. To achieve this target, simulations predicting the process results are necessary. An interesting process to simulate is the etching and rounding of pyramid tips in the ozone clean, where a diluted mixture of hydrofluoric acid (HF) and hydrochloric acid (HCl) is used for silicon wafer cleaning. The presence of ozone has an oxidizing effect on the surface cleaning, while the HF removes SiO_2 immediately from the surface; this leads to a slow etching in this process, which rounds the tip of the pyramid slightly (Fig. 3).

It is known from the literature [4], that these tip-rounding processes are useful in the production of heterojunction solar cells, since the round tip results in better passivation of the surface defects. A further understanding and optimization of the process in the given flow environment can help in optimizing the lateral homogeneity of the process. A process simulation for this etching process was therefore conducted. The model for the process simulation was built up from five pyramids which are located on the silicon surface. The flow of the process media was directed parallel to the diagonal of the pyramid base (Fig. 4, top). The simulation consists of a flow simulation in the volume considered and the transport of the diluted species in the circulated process solution, as well as the surface reaction, where O_3 and HF are consumed, while hexafluorosilicic acid (H_2SiF_6) is generated.

The etching process is isotropic with respect to the crystal orientations; therefore, the tip of the pyramid is attacked from several sides, while the pyramid surfaces are etched only from one direction. In consequence, the tip is rounded during this process (Fig. 4, bottom).

In addition to the qualitative result that the pyramid tips were rounded, quantitative results are also available. The dependence of the etching rate and the tip radius on the temperature and volume flow can be predicted using such a process simulation. The etching rate increases with increasing temperature as well as with an increasing volume flow, as seen in Fig. 5. Both effects also lead to a more pronounced rounding of the pyramid tips.

Empirical process modelling using artificial intelligence

The application of data-intensive deep-learning technology is promising for the quality control of high-throughput production in future PV fabrication. Fraunhofer ISE is working on a transfer of deep-learning algorithms to the levels of the PV value chain. A high-throughput characterization and production in the photovoltaic technology evaluation centre (PV-TEC) [5], and in cooperation

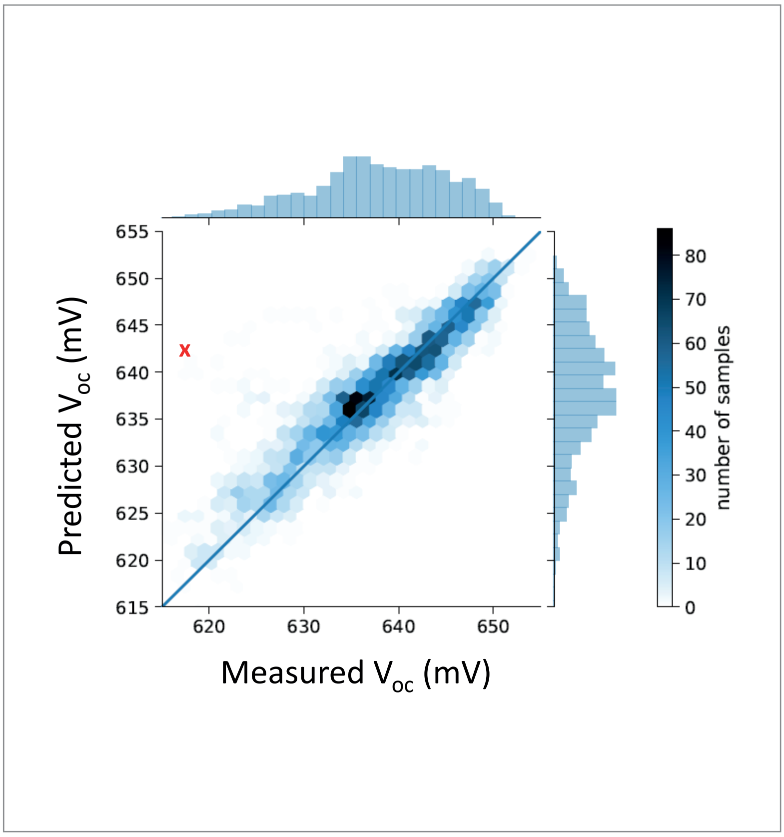


Figure 7. Predicted open-circuit voltage based on Fraunhofer ISE's deep-learning model; the red cross indicates an outlier, which is investigated in more detail.

with industrial partners, allows the collection of empirical data to establish reliable tools for predictive analytics and maintenance.

In Fraunhofer ISE's recent studies, a successful application of deep-learning algorithms for an inline quality rating of multicrystalline silicon (mc-Si) wafers was presented. Highly accurate prediction results allow the use of the model for fault detection. Nevertheless, machine-learning techniques are seen as a 'black box', which provides fewer physical insights. To broaden the acceptance of neural networks by the PV community, visualization techniques are presented here in order to help overcome any objections. Indeed, the network learns a semantic representation of the data, which can be used for defect analysis and localization.

Details on the leading application of novel machine-learning and visualization techniques for material characterization can be found in Fraunhofer ISE's studies on learning [6] and on visualization [7].

For mc-Si solar cells, the cell efficiency is heavily dependent on material quality. Crystallization-related defects – such as contaminations from the crucible, grain boundaries and dislocations – reduce the lifetime of the excess charge carriers. Lifetime-reducing defects can be observed in photoluminescence (PL) images [8].

Physical device simulations (e.g. ELBA [9]) can be used to predict the solar cell efficiencies from lifetime maps. Nevertheless, this approach is not well established for as-cut wafers before solar cell production: the lifetime of the excess charge carriers changes during thermal processes, and the measurement is limited as a result of the surface recombination of non-passivated samples. An empirical approach to rating the quality of mc-Si wafers using the novel deep-learning algorithms was therefore investigated.

A new era of machine-learning algorithms started in 2012: for the first time, machine-learning algorithms matched human-level performance [10] for the classification of a thousand different object classes in the ImageNet [11] dataset. Although the so-called *deep-learning techniques* have been known for decades (e.g. LeNet by LeCun et al. [12]), the breakthrough was delayed because of limited computational power and data. The emerging algorithms are fast and reliable. In an end-to-end manner, they directly connect high-dimensional input data, such as measurements during solar cell production, to quality parameters, such as solar cell efficiency.

A successful rating model can be established on the basis of known PL images of as-cut wafers and solar cell efficiencies. A sufficiently large amount of empirical data containing a huge material variation has been collected. PL images were measured during incoming control. The samples were processed within an industrial solar cell process for passivated emitter and rear cells (PERCs) [13]. The current–voltage characteristics (I–V) were measured for each sample, and pairs of corresponding data from incoming control and I–V data were identified through the marking of each sample with a data matrix code. A *convolutional neural network* (CNN) learns a mapping from PL images to I–V data on the basis of this comprehensive data set, as shown in Fig. 6.

For the model validation, the most complicated data distribution was defined: the test set contained only those samples from bricks (or even from manufacturers) that had not been used for the training of the model. The model validation showed a mean absolute error as low as 0.11%$_{abs.}$ for the efficiency prediction, and 2.0mV for the open-circuit voltage (V_{oc}) prediction, when materials of 'unknown' bricks were tested. A correlation graph for the open-circuit voltage is shown in Fig. 7. Comparable results were achieved for the prediction with 'unknown' manufacturers. The evaluation demonstrates the generalizability of the prediction model in terms of dealing with materials from different crystallization processes and feedstock variations.

"A generalized data collection opens up possibilities of using advanced data analysis and modern data science technologies and learn-from data."

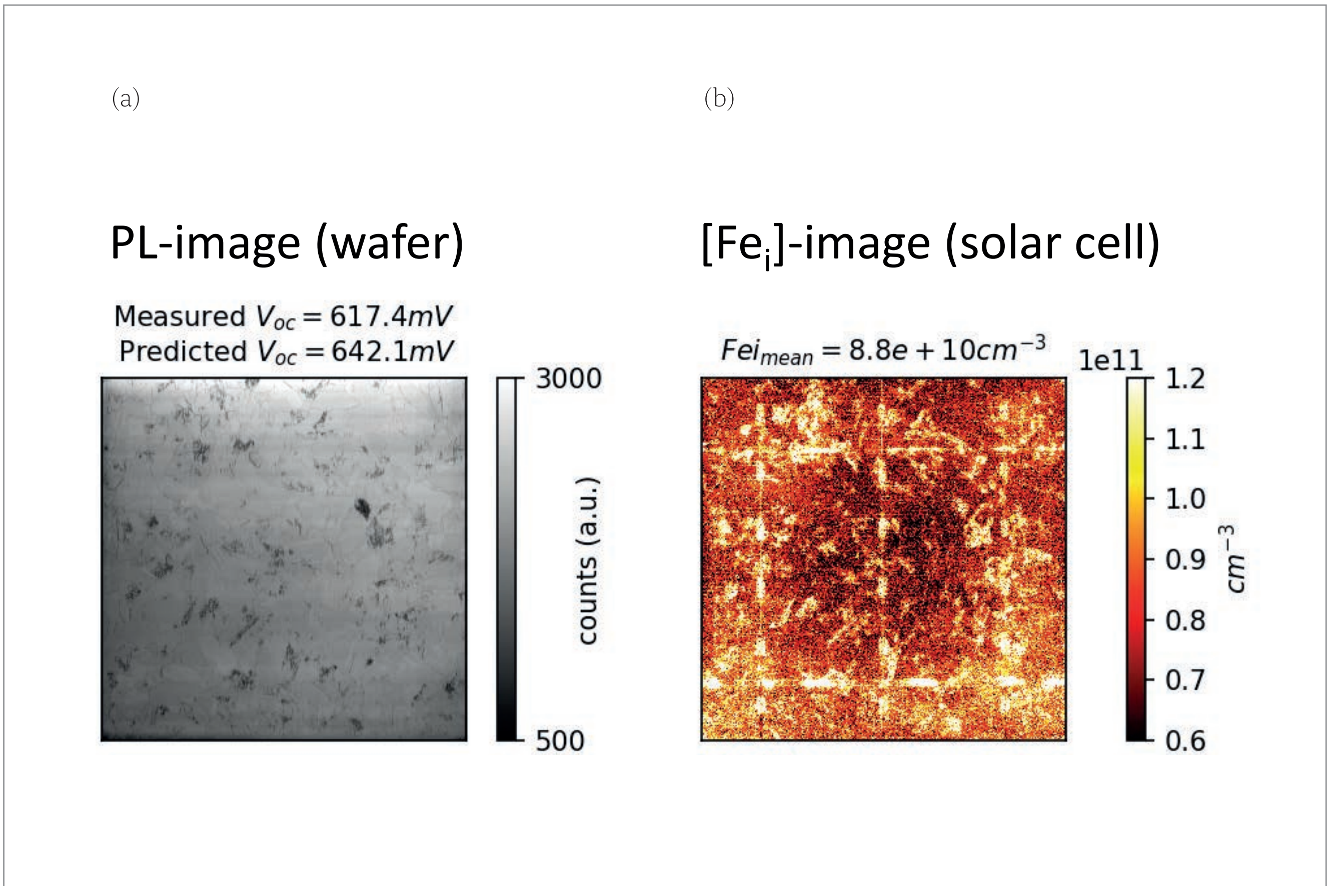


Figure 8. (a) PL image with a few visible structural defects, causing prediction errors. (b) The root-cause analysis reveals an increased iron concentration for samples with high prediction error.

Because of the high prediction accuracy, the network model can be used for fault detection and analysis. Deviations between predicted and measured quality parameters are indicators for process errors or variations in material quality, which cannot be observed in PL images. In the example here, a systematic overestimation of materials from one manufacturer was observed. For a detailed root-cause analysis of failure cases, advanced characterization techniques, such as the modulated luminescence (MODULUM) imaging method [14,15], can be utilized.

The data sample highlighted by a red cross in Fig. 7 was analysed in more detail. As illustrated in Fig. 8, the MODULUM technique reveals that prediction errors are correlated with an increased concentration of interstitial iron observed in the top regions of the ingot.

In the application under study, the CNN learns a direct connection between the 2D PL image of wafers and the *I–V* parameters of the solar cell. The end-to-end approach means that no expert knowledge needed to be provided to the model.

How do we know that we are right for the right reasons? To answer this, it is necessary to take a closer look at the network. By feeding a PL image into the CNN for open-circuit voltage prediction, the spatial resolution of the data is reduced at different stages of the network. The data are compressed to retain the relevant features, as previously shown in Fig. 6. The activations in the final layers can be combined to create an activation map and scaled to open-circuit voltage. It is now possible to localize regions of reduced material quality in the activation map which has been learnt by the network.

The network learns a semantically meaningful representation of the data which corresponds to the expectations of PV experts. Despite the low resolution at the final stages of the network, regions of reduced open-circuit voltage coincide with the crystallization-related defects (such as contaminated regions from the crucible and dislocations), as shown in Fig. 9. A comparison of the image of the dark-saturation current density (j_0) [16] of the solar cell with the activation map of the network for an input PL image of the as-cut wafer shows a striking similarity of the data.

Data flow in future production lines

Ideally, production lines correspond to the conventional automation pyramid, regarded as the so-called *industry 3.0* implementation. As a result, various communication systems, tailored to fulfil individual requirements, are in use in order to establish a highly structured vertical and horizontal data flow – taking into account all organization levels from the shop floor upwards through the whole company. The key business requirements that are to be met in this way exist on the vertical plane for all production planning and

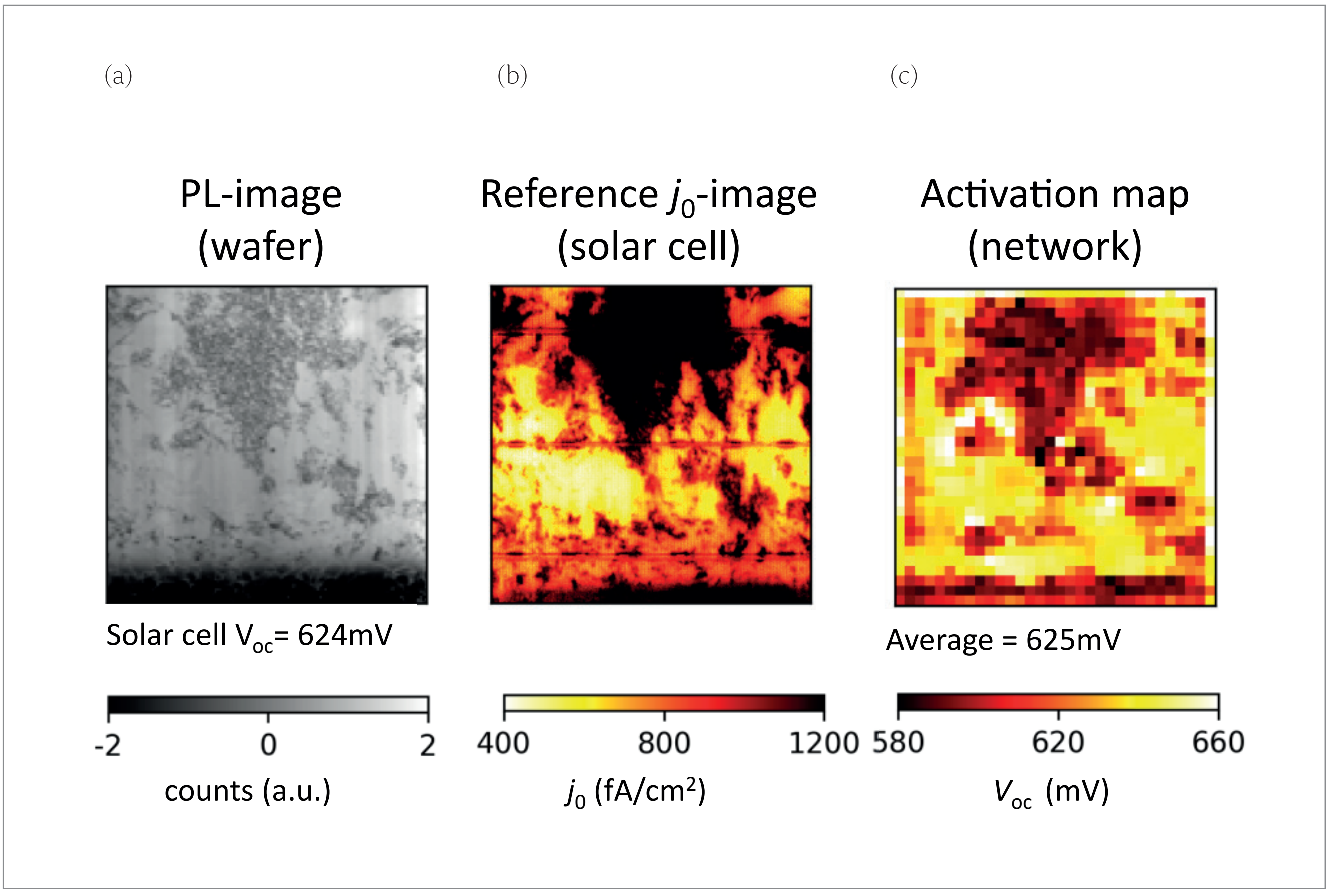


Figure 9. (a) PL image of the wafer, (b) image of the dark-saturation current density j_0, and (c) the calculated activation map according to the network model for the PL image in (a). The activation map reveals the expected V_{oc} distribution due to the material defects observed in the PL image and shows a high correlation with the j_0 image. The average activation value of 625mV represents the predicted result, which is similar to the measured value of 624mV of the solar cell.

data collection purposes, with a view to achieving general business objectives. On the vertical plane, only organizational and practical needs which contribute to fulfilling these vertical requirements are considered. The degree of digitalization and complexity of data flows in production lines are focused on these higher requirements and consequently only form reduced data structures with limited information value, such as stringent process specifications and conventional key performance indicators (KPIs). That typical approach leads production lines to keep almost 90% of industrially generated data decentralized, and to disclose only 10% of data which was previously declared to be important data.

In terms of industry 4.0 approaches, the data acquisition has to collect as much data as possible in order to generate a comprehensive pool of 'all data', without knowing or preselecting what is important and what is not, because that decision cannot yet be made at this point in this context. Because these data pools are meant to support a tremendous amount and variety of data structures, conventional data centralization and storage technologies need to be replaced by modern schema-less technologies. These technologies also enable concepts of distributed data pools and support dynamic data retrieval.

A generalized data collection opens up possibilities of using advanced data analysis and modern data science technologies and learn-from data. This is what is commonly regarded as *Big Data*; it makes all data accessible and allows learning from it. Whether it be simple data patterns or machine-learning results, it is the raw material for future product and process development and also paves the way to deeper process optimization in a more and more sensitive production environment. The main core idea is that not just data whose meaning and relationships are already known and deemed relevant are collected, but *all data* should be collected.

Of course, intensive data investigation and post-processing are necessary in order to extract new and relevant knowledge from Big Data pools. As soon as novel relationships become apparent in the data, appropriate data analyses can be standardized, simplified and introduced into production. However, the conventional requirements in terms of general business intelligence mentioned earlier must not be neglected and must be included in the new concepts from the start.

Data inherently require formalized structures that allow automated handling and ultimately allow processing and evaluation. Data of this type also form the basis of every digital communication – human to human, machine to machine, or human to machine. For centralization and organization, data are arranged in databases and permanently archived. In doing so, the database maps the formalized representation of the data in question through its database schema. The basic features of such a typically relational database are the standardization of the data structures that are fundamental to an application, the precision and consistency of the data in the database, and the routine of all operations within the database, as well as data exchange with applications external to the database. Usually, ERP and MES solutions are based on these approaches and are focused on these features as the main requirements to support business processes. All of these aspects are the strengths of a traditional, relational database system. However, these strengths are equally associated with limitations and restrictions when industry 4.0 concepts come into play. First of all, modern 'not only standard query language' (NoSQL) database technologies have to be integrated into existing business intelligence solutions.

The variety of different proprietary interface protocols for any type of digital communication also needs to be consolidated and unified. In addition, all components involved must be able to communicate bidirectionally with one another for intelligent communication. Open platform communication unified architecture (OPC-UA [17]) shows much promise for that purpose and is actually becoming a de facto standard for machine-to-machine communication. In contrast to the widely used SEMI PV02 interface, OPC-UA allows simultaneous communication with multiple clients; this enables a flexible implementation of several applications that can all access the data, which is provided in the entire production line.

Discussion and outlook

The fourth industrial revolution will change production technology in a sustainable way. Primarily, the rapid development of microcontroller technology, as well as the rapid drop in price of processors and memory devices, leads to an increasing variety of applications – from intelligent sensors and production tools to simulation models for the prediction of process results.

Empirical methods based on data-intensive deep-learning technologies are promising for the quality control of high-throughput production in future PV fabrication. Fraunhofer ISE's leading investigation was capable of modelling, on the basis of empirical data alone, the influence of material quality on the solar cell process.

One perspective on the acceleration of material development based on machine learning was put forward by Correa-Baena et al. [18]. Those authors propose that a balance between actionable results and inferring physical insights should be found in order to advance engineering and scientific objectives.

> "Digitalization as well as equipment intelligence, in combination with highly automated future GW-scale production chains, will represent the future of PV manufacturing."

It is assumed that this is especially true when it is a question of inline quality monitoring: a 'white box' model is not required for many characterization tasks in PV production, such as crack detection or even rating fracture strength, as long as sufficient data are available. Nevertheless, high predictability and physical insights are not mutually exclusive and can be tackled by developing methods for theory-guided data analysis.

Digitalization as well as equipment intelligence, in combination with highly automated future GW-scale production chains, will represent the future of PV manufacturing, offering interesting perspectives and technology differentiators for equipment manufacturers in the years ahead.

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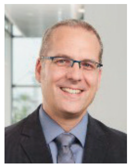
About the Authors

Martin Zimmer is head of the wet-chemical process technology group at Fraunhofer ISE. After finishing his studies in chemistry in Heidelberg, he received his Ph.D. from the Albert Ludwig University of Freiburg in cooperation with Fraunhofer ISE, where he investigated industrial texturization processes. His current research focuses on new wet-chemical production technologies in the context of industry 4.0.

Matthias Demant works on machine-learning techniques for material characterization and process control in the field of renewable energy at Fraunhofer ISE. He received his Ph.D. in engineering sciences from the University of Freiburg in 2016. As a postdoc he joined the vision group of the International Computer Science Institute (ICSI) at UC Berkeley in 2017. Since 2019 he has led a team involved in image processing and machine learning at Fraunhofer ISE.

Norbert Bergmann studied industrial engineering in Freiberg, and joined Fraunhofer ISE in 2008 to undertake his thesis on the topic of data management and analysis. Since 2010 he has been involved in the digitalization process for the Photovoltaic Technology Evaluation Center (PV-TEC) pilot line, and has been working in the fields of manufacturing execution systems and automatic data collection.



Stefan Rein is head of the quality assurance, characterization and simulation department within the PV division at Fraunhofer ISE. He studied physics at the Albert Ludwig University of Freiburg, where he obtained his diploma degree in 1998. He received his Ph.D. in 2004 from the University of Konstanz for his work on lifetime spectroscopy for defect characterization in silicon, and since then has been working in the PV-TEC at Fraunhofer ISE. His research at Fraunhofer ISE focuses on inline metrology, production control, machine learning, solar cell simulation and new silicon materials.

Jochen Rentsch is head of the production technologies – surfaces and interfaces department at Fraunhofer ISE. He studied physics at the Technical University of Braunschweig, obtaining his diploma degree in 2002. He then received his Ph.D. in physics in 2005 from the Albert Ludwig University of Freiburg. His work at Fraunhofer ISE focuses on R&D in rear-passivated solar cells and new wet- and dry-chemical processing technologies, as well as on coordinating cell technology transfer projects.

Ralf Preu is director of the photovoltaics (production technology) division at Fraunhofer ISE and also teaches photovoltaics at the University of Freiburg. He studied physics at the Universities of Freiburg and Toronto, and economics at the University of Hagen, Germany, and holds a Ph.D. in electrical engineering. He joined Fraunhofer ISE in 1993 and has worked in different fields in PV, including system monitoring, silicon solar cell and module technology, characterization and simulation. His main focus is R&D in advanced silicon solar cell technology and its transfer to industrial production.

Enquiries

Email: martin.zimmer@ise.fraunhofer.de