Data Guided Materials Processing - Digital Material Twin and Digital Material Shadow

Concept for databased Material Property Description along the Process Chain

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Abstract

A digital twin is a virtual representation of a corresponding process of a physical object. In context of industry 4.0, a digital twin provides new opportunities for production optimization and failure prediction. Therefore, both industry and scientific research show increasing interest in digital twins. One of the most important sectors in the production value chain is material science, which plays a very important role for the product properties and processing strategies. However, the digital microscopic and macroscopic description of materials' properties and its processing are currently not fully defined. Therefore, in order to implement materials into the digital representations of production processes, a throughout digital description of the material and its properties – a digital material twin – is presented in this paper. An extended digital material twin is further defined and includes the processing history. Thus, a throughout description of the material is enabled. The extended material twins can be connected to a process chain. Thus, we describe the concept for a comprehensive description of the materials' properties within the production value chain. For more complex, data intensive, descriptions, a concept to reduce the data, the digital material shadow is introduced as well. Our approach defines a framework to thoroughly describe a material and its development during processing or production.

1. Introduction

In recent years, digitalization, data-driven approaches and database applications has drawn attention particularly in traditional manufacture industries [1]. Concepts for digitization of a physical process like a cyber physical system, allow a sensor-based monitoring and increase control of industrial process chains [2]. However, an optimization of the analyzed systems is only possible when the collected datasets are correlated by the system in real-time during the production process. Thus, the datasets and their mutual physical interdependencies should be described within the cyber physical system. Therefore, a domain knowledge, so called *Digital Twins (DT)*, can be used. The concept of a DT was originally introduced in 2003 from Grieves et al. [3]. They described the DT as a digital representation of a physical product and divided it into three main parts: (i) the physical object, (ii) the digital replication and (iii) the data and information which connects both (**Figure 1**) [3]. The DT evolved during recent years is a dynamic digital replica of its physical counterpart [4] and a powerful tool to represent, monitor, diagnose and prognose a system, a production line, an object or a service [5]. The application of a DT efficiently helps from urban planning of smart cities, to support in the healthcare industry to improve the effectivity of certain drugs, or planning, performing and simulating surgeries [5-7].

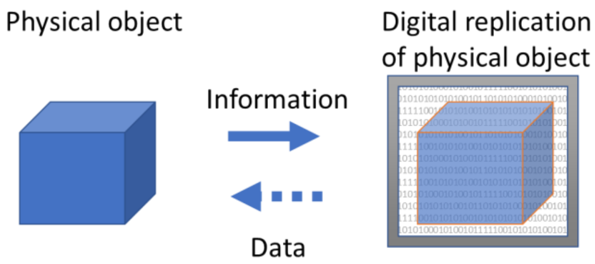

Figure 1 - The concept of a digital twin

Publications and patents dealing with the DT from 2003 to 2018 were reviewed by Tao et al.[5]. They found that the DT is used in several industries, for example design, production, prognostics or health management. Especially in production engineering, the DT has a great impact. The DT of production describes the full use of the relevant data from equipment, environments and history data from the previous generation of the products. This enables predictions on the product quality even before production takes place, hence the R&D resources for the product evaluation process can be reduced. One of the most important advantages of the DT is the information on the status of machine performance and production line feedback in real-time [6]. Compared to the traditional manufacturing, the DT provides an environment for product and system testing, which gives the manufacturer opportunities for predicting the issues before or during the production [10]. This optimization leads to improvement of the process plan control [9]. The DT can also be used to facilitate the production optimization. Uhlemann et al. presented a multimodal data acquisition and evaluation concept and proposed guidelines for the implementation of the DT to optimize production systems [11]. These are the basis for the Prognostics and Health Management (PHM), which was first applied in aircraft industry. Tuegel et al. summarized the current aircraft structural integrity and life prediction concepts and proposed a DT-based life assessment strategy, which enables a better management of an aircraft-life series and a full-scaled data collection of the conditions of the aircrafts at any time [12]. Moreover, the digital twin approach can promote the adjustment of production operations based on both practical situation and simulation [13]. Bielefeldt et al. proposed a digital twin-based approach which can detect, monitor and analyze the structural damage of commercial aircraft wings by taking the applied material into account and placing it into the focus of the model [14]. The digitalization of new material design has been pushed by various scientists. The open-sourced material database projects, such as Japan's National Institute of Material Science [15] and Material Genome Initiative [16], which includes experimental and computational results of materials, provide the researchers the benefits for material data sharing, material sorting for specific purpose and new material design. However, the information of material processing, which includes the history of the material state, is not provided in those approaches. With the shortage of this information, a throughout digital material state description is difficult to provide and the application of the digital material description in production is also challenging.

If we consider the material as the core of a processing chain, then the metadata which represents material properties from each processing step should be collected, analyzed and stored. Eventually, the analyzed results should also be applied as for digital description of material during processing and the results from individual processing steps should be connected for the representation of material in the processing chain. Moreover, in the processing chain, the change in material properties needs to be correlated to relevant datasets during processing. To fulfill the mentioned requirements and build up a comprehensive description of material development, the concept of a *digital material twin* (DMT) has been introduced and refined within the last years, to describe materials and its changes due to the processing steps.

In addition to the concept of DMT, we will further introduce the Digital Material Shadow (DMS), a concept to reduce the complexity of DMT. Based on Platon's alegory of the cave, the shadow reduces the information of the physical object as only a 2D representation of its shape and movement are remaining (**Figure 2**). Hence, the shadow can be considered as a representation of certain characteristics from a specific point of view, e.g., changes in the rolling forces on material-intrinsic temperature responses.

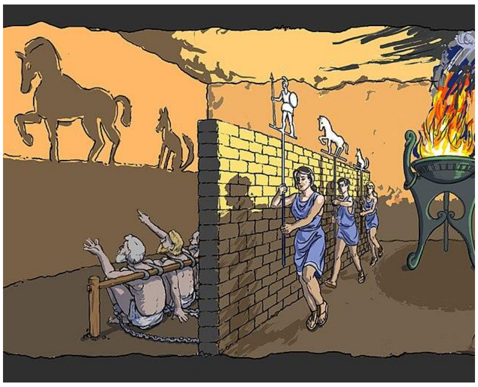

Figure 2 - Illustration of Platon's *allegory of the cave* - the shadow as a representation of the physical world [17]

2.1 Digital Material Twin

Before the DMT is defined, we first define a substance or a mixture of substances that constitutes to an object as a *material*. The most important engineering materials are metals [19]. Today, steels have the highest technical significance of all materials with respect to production volume and variety of application. Accordingly, our following definitions describe steels, but can be extended to other materials such as ceramics, semiconductors and polymers. In general, material properties are not equal to the properties of a workpiece (the **extrinsic properties**), since the shape, roughness, stiffness etc., can have controversial correlation with the properties of the material itself (the **intrinsic properties**). Furthermore, the intrinsic properties are the reflection of the phase state (phase type, distribution and fraction, etc.) of a material, which is as well the reflection of the crystal lattice structure. Therefore, the first step for the DMT definition is to distinguish the intrinsic and extrinsic properties and excluding the extrinsic from all available information on the current state of a material (as shown in **Figure 3**).

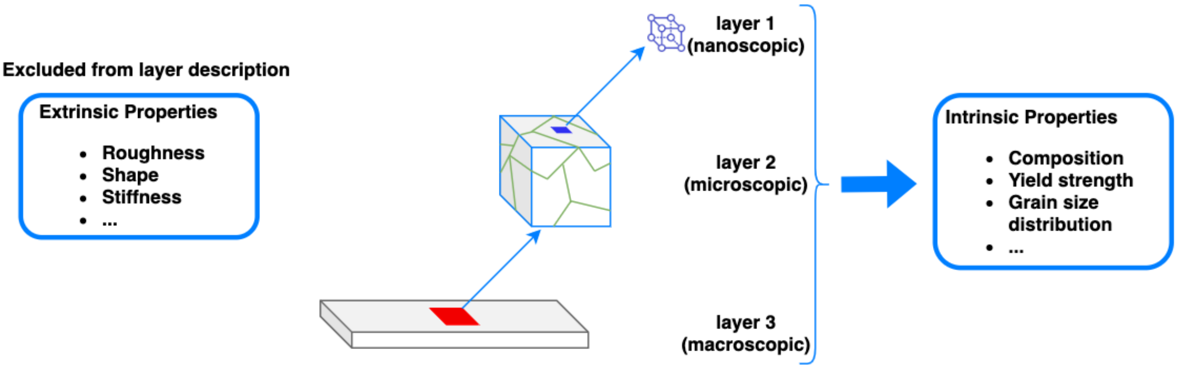

Figure 3 - Differentiation of exterior properties of the workpiece (extrinsic properties) and material properties (intrinsic properties)

The intrinsic properties describe the current state of the material and reflect the crystal lattice structure and phase information. Therefore, **Figure 3** can be used as an example, which is divided into **three layers**. In **layer 1**, the nanoscopic description of material will be considered. In this layer, a description from atom point of view will be presented, in which the crystal structure and the crystal defects, distribution and diffusion of foreign atoms are described. This information is strongly correlated to the description in the following layers and have enormous impact of material properties in layer 2 and layer 3. Therefore, the nanoscale layer (layer 1) is the fundamental layer and the information in this layer should be provided for the following layers.

layer 2 and **layer 3** hold information of layer 1 and describes the material by its phases and further microstructural characteristics, like phase fractions, orientations, grain sizes and grain size distribution. An example is given in [18]. The local chemical compositional of C and Mn and microstructural parameters of complex phase steel CP800 are correlated and quantified, which provide a comprehensive and as well a quantitative description of layer 1 and layer 2 (**Figure 4)**. Moreover, the approach provides the possibility for the description of the correlation between different intrinsic properties and leads to the comprehensive DMT construction.

Furthermore, **layer 3** of the metal can be considered as a statistic summary of all the unit cells in layer 2, e.g., the Young's modulus of the material in layer 3 can be considered as the average value of each unit cell from layer 2. Hereto, a 3-layered description is sufficient for the metal property description, which can be defined as **intrinsic property** of the material, as mentioned above.

However, in all three layers, the properties which are related to the work piece (shape, roughness etc.) are neglected. If the material is applied in production, the properties which relate to the work piece should also be considered, therefore, the intrinsic properties and the properties of the work piece needs to be correlated. Therefore, we define the work piece properties as **extrinsic property**, which are excluded from the 3-layer description of material, as shown in **Figure 3**. Furthermore, the description of extrinsic property can also be applied for cross domain connection (or the combination of other Digital Twin in the production). However, a 3-layered description of intrinsic properties is sufficient for the material description, therefore, a detailed introduction of extrinsic properties and the correlation between intrinsic and extrinsic properties will not be presented in this work.

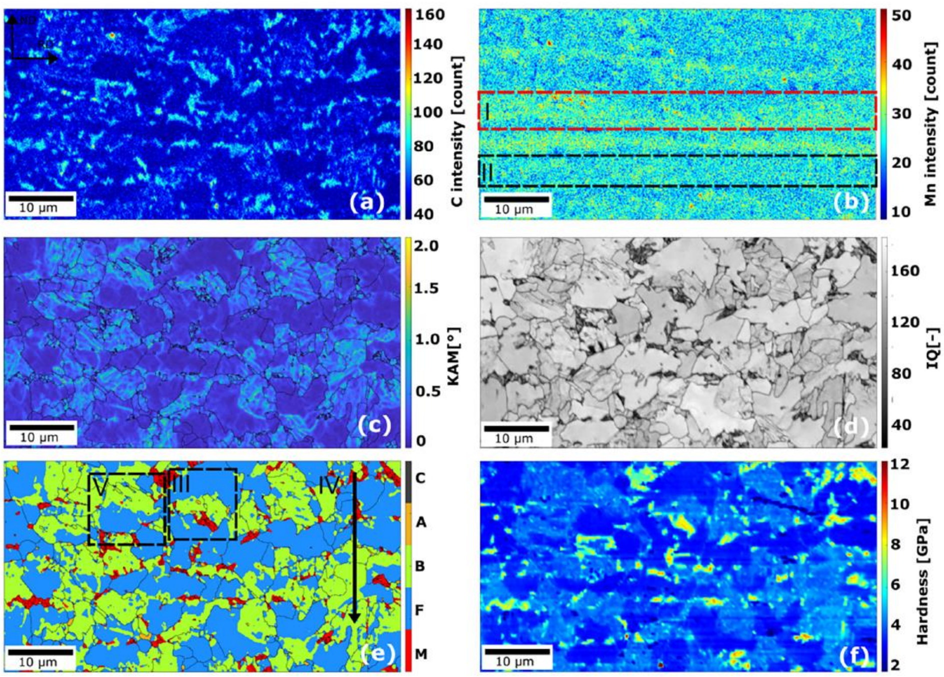

Figure 4 - One example of correlation between hardness, microstructure and local chemical composition from [18]. The correlated EPMA, EBSD and hardness maps over a 64 × 32 μm area of CP800 steel: (a) C intensity map (unit of counts), (b) Mn intensity map (unit of counts), (c) Kernel average misorientation (KAM) map (3rd nearest neighbor), (d) image

quality (IQ) map, (e) phase map defined by IQ and KAM criterion, (f) hardness map. Grain boundaries (θ > 5°) are represented by black lines in (c)-(e).

Therefore, a material can be digitally described by this three-layered model with a high variation of parameters for a certain state. Moreover, the specific layers are correlated with one another, as shown in **Figure 5**. This digital description of the materials' intrinsic properties can be defined as ***DMT***, which represents the material in the virtual space. Furthermore, a simulative description should also be considered as a part of the DMT, making it possible to use the combination of physical and simulated datasets to increase the informational content, which further reduces the need for testing procedures [3]. To describe the change in material properties in a process chain, it is important that any process stop is connected to the previous (and subsequent) process steps. Since the DMT is a description of the material state which may change along the process chain, a DMT has to be described for each process step.

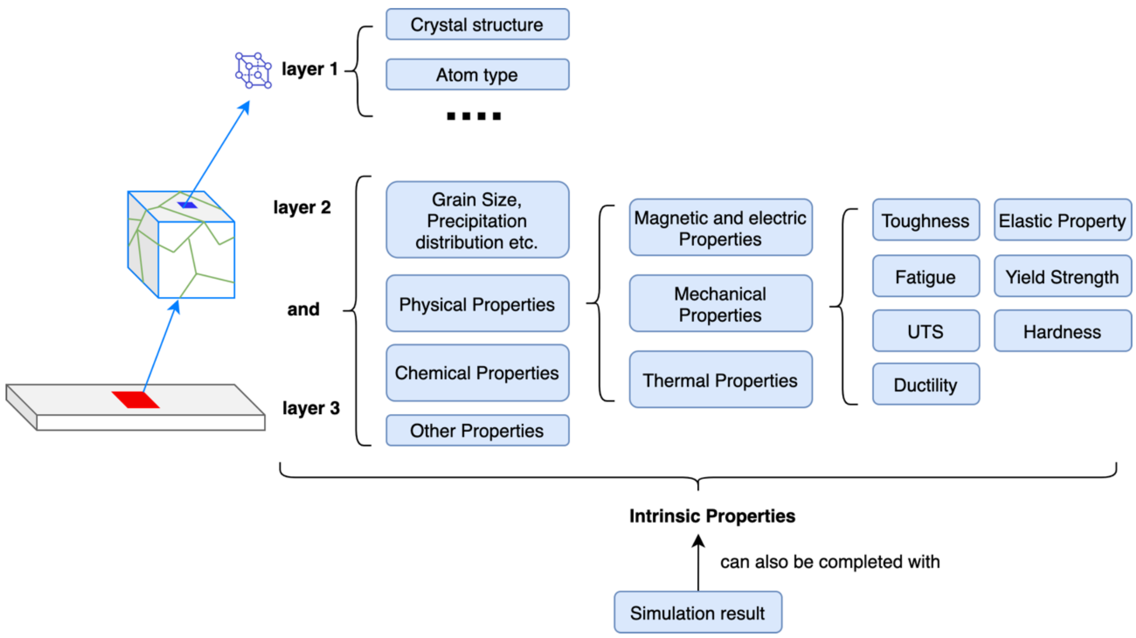

Figure 5 - Schematic illustration of DMT: the intrinsic properties, which are irrelevant to the workpiece in 3 layers of one DMT

To describe the connection of the DMT and the process, we need to extend the DMT. The extended DMT (eDMT) is shown in **Figure 6** and includes the processing that resulted from the DMT. Moreover, the material state change in one processing chain can be described by connecting all the relevant eDMTs, as shown in **Figure 7**.

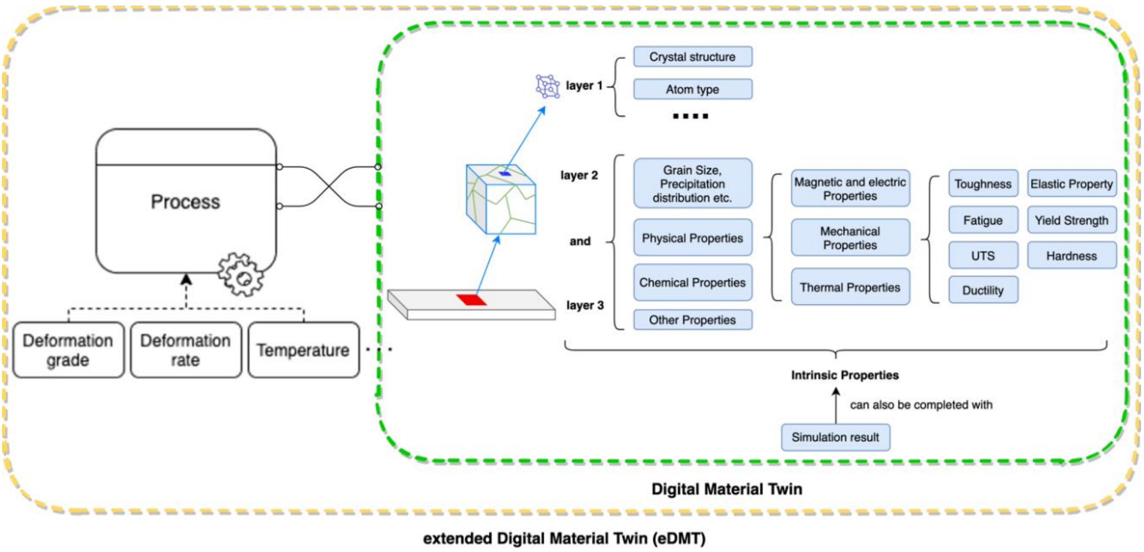

Figure 6 - The DMT, which is extended with the correlated processing parameter (eDMT)

In **Figure 7**, the concept of the eDMT is used to describe a simple process chain (and all the eDMTs in this process chain form one **Digital Process Chain**), which includes a rolling process and a subsequent annealing process. At the beginning of a process chain, occasionally no "preprocessing" is given, so we can also start the process chain with a DMT. Furthermore, certain properties of the DMT change within the process (while others remain). At first, the raw material goes through a rolling treatment to adjust its mechanical properties for the application. In this process, the overall chemical composition of the material remains the same, while parameters like dislocation density and the shape of grains change, in relation to the processing parameters. The same is valid for the subsequent annealing process, where again some parameters change while others remain constant. This shows that several parameters are connected along the process chain. For each eDMT within the process chain, a high variety of properties can be evaluated or simulated. This leads to a high complexity when the eDMTs need to be connected to one another, and correlations need to be found. In order to identify correlations, numerical, analytical or data-based models can be used. However, for controlling material state variation during processing in real time, a highly efficient data-based model needs to be designated and evolved for specific aspect from the material, by which the relevant datasets and the model for the dataset-correlation within each eDMT will be selected and collected; in other words, the eDMT must be reduced. This new data-based model can be applied not only for monitoring of the target intrinsic properties, but also for the material-science-based diagnostic of the target property deviation and adjustment, as well as prognostic of the target property based on the processing parameter and history information. Furthermore, data exchange between this model and the models from other knowledge domains in production technology (e.g. the model for above mentioned layer 3 in production) should also be taken into consideration. Therefore, apart from eDMT, we propose another concept for the material digitalization in the production, the *Digital Material Shadow* (**DMS**).

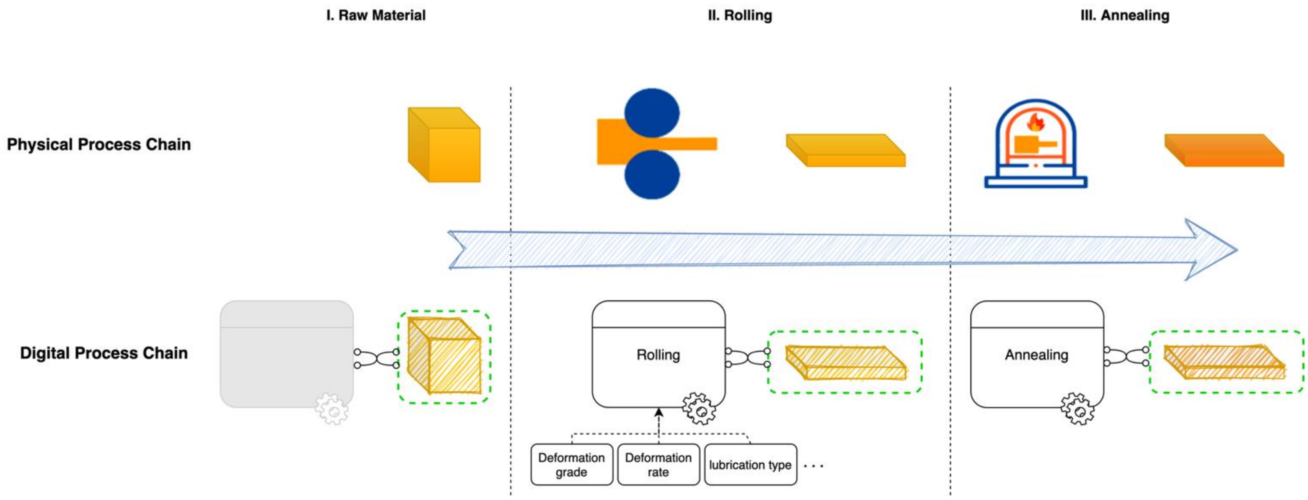

Figure 7 - Comparison of the Physical Process Chain and Digital Process Chain (formed by three (e)DMTs)

2.2 Digital Material Shadow

In one production process, one intrinsic property of material is important and needs to be monitored, which will be defined as **target property** in the following discussion. This target property of the component is influenced not only by the treatment parameters during the process, but also affected by the fluctuation of other relevant material properties itself. First of all, the dataset of processing parameters and the sensor-collected dataflow of temperatures, forces, etc., which are correlated to the target property, must be automatically defined and correlated throughout the processing, while the irrelevant processing parameters should be ignored. Furthermore, if a detailed eDMT would be set up, the size and the complexity of the dataset collections of the eDMT would be enormous, e.g., for a 10 µm grain size material each mm³ would require a complex CP-FEM treatment of 1 million grains throughout the processing steps. Therefore, for one production process with respect to target property, the relevant datasets from eDMT should be correlated. Thus, we use the term “shadow” in analogy to Platon’s allegory of the cave as a reflection of the object characteristic and introduce another concept: The *Digital Material Shadow* (DMS) as an interaction approach of the reduced eDMT model and external sensor dataflow, which will be introduced in the following chapters.

2.2.1 Definition of Digital Material Shadow

In chapter 2.1, we defined DMT as a 3-layered description of a material intrinsic property. Furthermore, if one property is selected as target property and set as observation point of the DMT, the correlated datasets should be extracted for the description of the characteristics of DMT under this certain observation point. Taking **Figure 4** (cf. [18]) as an example, the target property of the DMT would be considered as hardness. In this case, for one single unit, the mechanical property was applied as one observation point, afterwards, the extracted properties (in this case, chemical composition and information of microstructure, e.g. grain size, phase fraction, precipitation etc.) and the correlation between target property and extracted properties were presented for the description of DMT’s target property for this single unit. One example of the correlation in this case is the Hall-Petch relation [19], which describes the correlation between yield strength and grain size.

With the addition of the single unit, the target property of the material is described. Furthermore, with application of artificial intelligence (AI) approaches, more potentially unknown correlations can be identified. Thus, more datasets and correlation models (apart from chemical composition and microstructure) from different layers can be introduced.

Moreover, if the observation point is changed, the different properties would be presented from layers. E.g., if the phase fraction were considered as one aspect, then from all 3 layers, the correlated models and datasets (e.g. heterogeneity of chemical composition, crystal structure and information of precipitations etc.) would be observed, as shown **in Figure 8.**

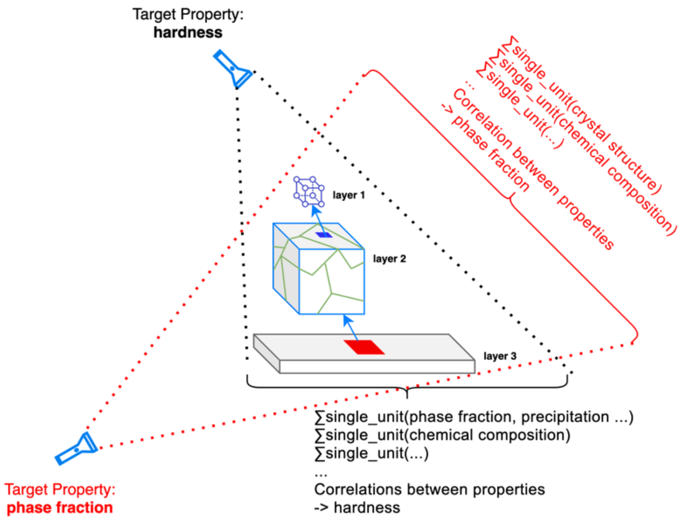

Figure 8 - Correlation for determination of target property: hardness (black) and phase fraction (red), ∑represents the summarization of different properties in one unit

Furthermore, if the extensions are considered, then not only the parameters of the treatment, but also the datasets, which are collected by sensors during the processing, must be included into the reduced model. One example is the hardness as target property from **Figure 8**. The processing area is considered as one monitoring area of one eDMT. Furthermore, in this monitoring area of eDMT, one sub-monitoring area is further divided with monitoring range of one sensor (here, the sub-monitoring area is defined as single_unit). Through the target property (e.g. in **Figure 9**, the hardness during processing), a dataset collection (chemical composition, microstructure, etc.) from different layers of DMT is created and correlated with processing parameters (time, temperature, force and atmosphere etc.) from the extension for the description of the microstructure changes (or phase transformation) during the process. Subsequently, the correlation between the material properties and the processing parameters will be analyzed and applied as models for the DMS description. One the one hand, with the approach introduced in [18], or the other empirical/physical models, the correlation between hardness, microstructure and inhomogeneity of local chemical composition can be described (same for other mechanical properties, e.g. for yield strength, Hall-Petch relation, which is applied for correlation between chemical composition, grain size and yield strength). Hence, for this single unit, the material property change, which is observed, can be correlated to various deviations of material properties from all three layers. On the other hands, the changes of the processing parameters which are collected by the sensors and the correlation between parameters and material properties will be analyzed. E.g. the impact of the temperature fluctuation on local chemical composition due to diffusion can now be analyzed and quantified. This impact can further be transmitted to other correlated properties with help of the above-mentioned models. With these correlations, the target property can be manipulated through adjusting processing parameters or the other correlated material intrinsic properties, as well as prognosing through pre-given parameters.

If all the single units are integrated as one collection, then the whole effective processing area of the treatment is described as one digital trace (with respect only to the material properties and treatment parameters, which are correlated with the observed material properties) of one material processing (see **Figure 9**).

Therefore, a DMS can be defined as one reduced model of DMT or eDMT for the observation of target property of the material, analogously to the shadow in **Figure 2**, which reflects the characteristics of the physical object. Moreover, the DMS can be applied along the process chain (or the eDMT chain) for the monitoring and, with help of AI or data science approaches, for diagnostics or prognostics of the target property.

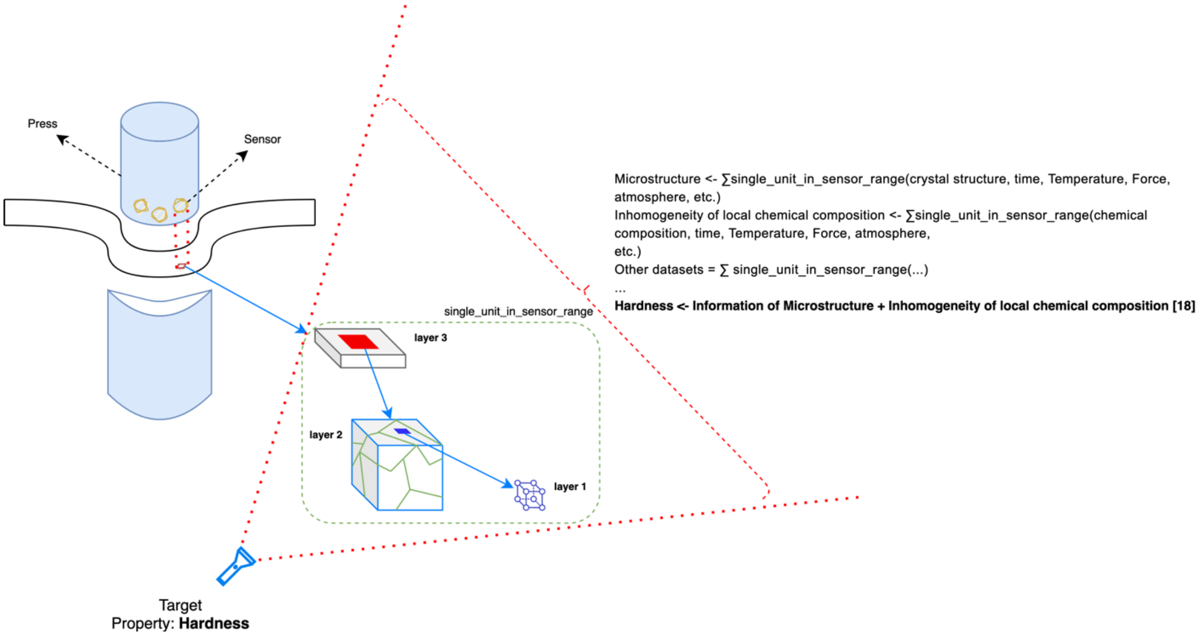

Figure 9 - Schematic illustration of eDMT observation with target property “hardness”

2.2.2 One Use case of DMS in Internet of Production (IOP): Press Hardening

In this chapter, press hardening is selected as one example for DMS application. One of the products which will be produced by press hardening is B-pillar. For material of B-pillar, one of the most important properties is the capacity to dissipate energy are important aspects for the protection of passengers in the event such as site impact or rollover. Therefore, the mechanical properties of the material such as tensile strength (R_m) and hardness are of interest and should be monitored, diagnosed and prognosed during the press hardening process. Here, we take tensile strength (R_m) as an example and defined as one Target Property for the following definition. With help of the 3 layered description of the DMT, 2 intrinsic properties which are correlated to the target property are taken out (chemical composition and microstructure information).

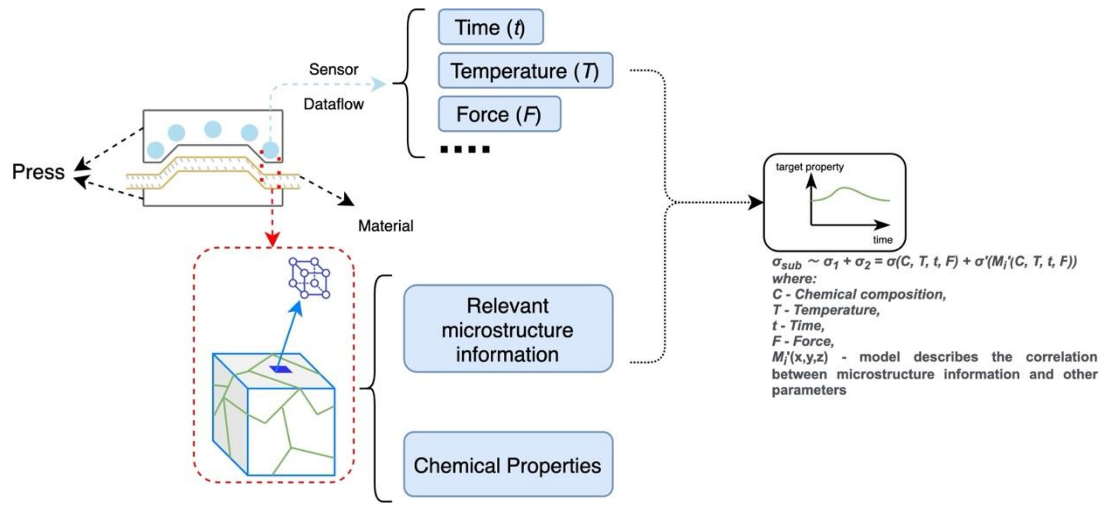

Figure 10 - Schematic illustration DMS of Press hardening: target property monitoring through reduced eDMT and dataflow collected by sensors

As shown in **Figure 10**, the sensor which monitors one sub-area of the material, collects the information of the local chemical composition (or shows the heterogeneity of the chemical composition in this area). Furthermore, the dataflow which represents the temperature (*T*), time (*t*) and force (*F*) in this area are also collected by the sensors. If the first layer of eDMT is considered, then the atom behavior (both substitutional solid solution atoms and interstitial solid solution atoms) during the processing will be correlated to the sensor collected dataflow (*T*, *t* and *F*), and the tensile strength from the first layer can be described with the following correlation:

$$\sigma_1 \sim \sigma(C, T, t, F) \qquad \textbf{(2.1)}$$

where C represents local chemical composition. Moreover, if we consider the second layer of the eDMT, then the relevant microstructure information (M_i) of this monitored area can be predicted by implementing time-dependent dilatometer data, and with help of the *T* and *t*, with the following correlation:

$$M_i \sim M_i(C, T, t) \qquad \textbf{(2.2)}$$

where C represents local chemical composition. Moreover, the microstructure can also be affected by the implementation of the force, *F* (e.g. strain-induced martensite formation and dislocation density) and the interactive effect of *F*, *T* and *t* (e.g. recrystallization). Therefore, the correlation (2.2) can be rewritten as followed:

$$M_i \sim M_i'(C, T, t, F) \qquad \textbf{(2.3)}$$

Therefore, the tensile strength in the 2nd layer can be described as followed:

$$\sigma_2 \sim \sigma(M_i'(C, T, t, F)) \qquad \textbf{(2.4)}$$

Eventually, the tensile strength of this sub-area can be described as the summary of both σ_1 and σ_2:

$$\sigma_{sub} \sim \sigma_1 + \sigma_2 = \sigma(C, T, t, F) + \sigma'(M'(C, T, t, F)) \qquad \textbf{(2.5)}$$

If all the sub-areas, which are monitored by the individual sensor, are considered, then the target property (in this example, tensile strength) is monitored and can also be prognosed by the dataflow collected by the sensors. In this case, the DMS is created by the collaboration of reduced eDMT model and the sensor-dataflow in real-time, which represents the target property change during the processing, as shown in **Figure 10**. The DMS also provides the opportunity for the real-time manipulation of the target properties: if the range of target property is defined, then the parameters:

T, *t* and *F* can be adjusted for the designated target property. Furthermore, if the measured property of the material exceeds the range of the target property, then the target property deviation can be backtracked through parameters (e.g. *T*, *t* and *F*) or other correlated intrinsic properties for main cause of the problems (diagnose).

3 Conclusion and Summary

In this work, two concepts for digital material description are introduced: digital material twin (DMT) and digital material shadow (DMS). A DMT describes the material state by providing its intrinsic properties which are not relevant to the workpiece (which are defined as extrinsic properties in this work) and correlation in 3 layers along the material length scale (nanoscopic, microscopic and macroscopic) with help of both experimental and simulation datasets. Furthermore, the DMT is extended as eDMT with the parameter dataset of the material processing, which leads to the subsequent DMTs in the processing chain. A material state change in one processing chain can be described by connecting all the relevant eDMTs (eDMT chain). DMS is introduced for reducing the data complexity of eDMT or eDMT chain, which also provides the possibility of material state monitoring in real-time during the processing. The monitoring function can be realized through the reduction of the eDMT to target property and the implementation of the sensor dataflow in real-time. The target property can further be diagnosed and prognosed with help of AI or data science approaches. Moreover, DMS is applied on the process of press hardening, in which the target property is monitored, diagnosed and prognosed with help of the correlation models with intrinsic properties and collected sensor dataflow. A deep collaboration of experts in relevant fields enables an efficient design and application of eDMT and DMS.

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Conflict of Interest

The authors declare no potential conflict of interest.

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