Graph based process models as basis for efficient data driven surrogates – Expediting the material development process

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Abstract

Shorter development cycles, increasing complexity and cost pressure are driving the need for more efficient development processes. Especially in the field of material development, the long and costly experiments are a major bottleneck. To alleviate this, data driven models, supporting the decision making process, have recently gained popularity. However, such models require a structured representation of the development process to allow an efficient training. In this work, a formalism for deriving an efficient representation of material development processs (MDPs) is proposed, shown exemplary on the development of a high modulus steel (HMS). The formalism is based on the combination of graph based process models and the recently proposed concept of "flowthings". This allows to efficiently derive a directed acyclic graph (DAG) representation of the MDP with the acquired data. From this, a database for subsequent training of surrogate models is derived, on which several black box models for the MDP are trained. Best-in-class models are chosen based on the root mean squared error (RMSE) on the test set and substantially used for the inverse optimization of the MDP to maximize the specific modulus while meeting additional design constraints. This

showcases the potential of the proposed formalism for expediting the MDP by enabling data driven modeling.

Keywords: Process development, Surrogate modeling, Data driven decision making

1 Introduction

Increasing environmental and economical requirements accelerate the development of novel technologies in the aviation industry [1]. This lead to a significant growth in aircraft turbines overall but especially their bypass ratios [2]. The resulting loads, which the turbine has to withstand, are so high that conventional materials cannot be used anymore.

Hence, novel steel alloys with significantly increased specific Young's modulus, so called HMS, are being developed for the application in high bypass ratio turbines. One approach that is being thoroughly investigated since 25 years is the formation of microscopic ceramic particles that are embedded in the metallic matrix [3–6]. Especially the in-situ formation of the reinforcement particles is highly desirable, since it allows the reduction of the number of process steps required until up to the final product. This, however, introduces additional complexity, which, despite the substantial research effort, is still the focus of current research [7, 8].

To better understand processes and inherent interdependencies of the plethora of process parameters, the consistent monitoring and modeling of processes has been a promising approach. Based on the structured foundations of product development processes, i.e. summarized in [9], and the principle of an interactive design process [10], process models have been proposed by many authors. Zhang et al. extended the Vee-cycle to a system engineering base "innovative design model", that combines static requirement analyses with dynamic response possibilites [11]. Schabacker et al. streamlined business process model and notation (BPMN), design structure matrix (DSM) and a container model into one coherent solution, supporting the optimization of modeled processes [12]. Stanković et al. proposed the representation of process chains by directed multigraphs, incorporating expert knowledge by newly developed graph grammar rules [13]. Khodabandelou et al. point out the importance of taking the intention behind the modeling effort into account from the beginning to significantly enhance the efficiency of the modeling process [14]. They leverage the intent for automated process mining from logged information, leading to a fine-grained representation of the observed processes which is coarse-grained in a second step, introducing a higher level of abstraction. Jin and Liu proposed an extension of process monitoring, and thus the basis of its modeling, for multistep processes with inherent parallelisms [15]. Al-Fedaghi proposed an alternative to the BPMN by focusing on so called "flowthings", general objects that are passed from one process step (PS) to the next and are processed in each PS they pass [16]. Zitzewitz and Fieg showcase how a reliable process model can enable the optimization of the underlying process and thus deepen the understanding thereof [17]. Haider et at. subdivided individual process steps into

related model, method and data, to further modularize PSs and thus formalize the interface between individual PSs [18].

In recent years, the usage of data driven models to tackle complex tasks to save on expensive experiments or simulations has become increasingly popular in the fields of engineering and materials science. Tao et al. used Gaussian processes (GPs) to optimize vehicle suspension for dynamic stability [19]. Sun et al. compiled a review on the application of artificial neural networks (ANNs) as surrogate model in the design of aerodynamic parts [20]. Hadidi et al. used a response surface model for reliability analysis in high dimensional spaces [21]. Teng et al. approached a similar challenge by training a model capable of assessing a system's reliability by adding generative adversarial theory to surrogate models [22]. Yan et al. employed a combination of GPs and physically based methods to predict the mechanical properties of additively manufactured alloys based on their composition and process parameters [23]. Building on accurate models that can predict the results of a given process, there has been research effort to flip this approach and utilize the inherent knowledge in order to adapt the process to obtain desirable results. Jiang et al. used surrogate models for the optimization of designs [24]. Gerritzen et al. proposed a constitutive model for the out of plane shear behavior of fiber reinforced polymers derived from pure data analysis [25]. They further facilitated its usage through an ANN based method for direct parameter identification, capable of extracting the material parameters from experimental stress-strain curves in one step [26].

Fürstenau et al. used smooth particle hydrodynamics (SPH) simulations to obtain a virtual process map of an selective laser melting (SLM) process [27]. This was necessary due to the high dimensionality of the parameter space the SLM process spans. Similarly, Vohra et al. used simulation data as basis for surrogate model training. They, however, combined the simulation with dimensionality reduction techniques for best performance and sensitivity analyses [28]. Hürkamp et al. ran detailed process simulations to obtain a good understanding. The results were trained into surrogate models, which were used to transfer the gained knowledge to the operational phase [29]. Pfrommer et al. did some process optimization using ANNs as surrogate models [30] via iterative training on simulation data.

With the task of setting up a process comes always the challenge of of efficiently finding a good set of parameters. Especially in high-dimensional cases, classical design of experiment (DOE) approaches may lead to an unreasonable number of tests necessary. In the additive manufacturing example [28], the input dimensionality is 12. Using factorial based DOE algorithms, this would lead to a total of 128 (full factorial, 2 steps) 4120 (central composite). Even though such approaches can give good insights into the overall process behavior, their rigid form, i.e. not taking results from previous tests into account, can lead to suboptimal DOEs.

Therefore, so called sequential experimental designs have been the focus of many studies. Thompson laid the foundation for this in 1933 with the suggestion of even taking information from two data points into account for further experimental planning [31]. This idea was formalized in the 1950s , i.e. by Bellman [32] and Chernoff [33]. Since then, it received continuously increasing research attention, i.e. [34–36]. Since 1990 the number of publications every year focusing on this challenge has started

accelerating quickly [37]. This underlines both its importance but also the complexity and lack of final solution.

In this work, an approach for modeling a real world material manufacturing process of an HMS, consisting of multiple steps, is presented. The goal is to transfer influential parameters into a representation that can be used for subsequent training of a surrogate model. Here, several models are compared and the "best-in-class" version is chosen for final analyses. The chosen model is used for the efficient optimization of the overall process objective, i.e. maximizing stiffness while meeting other design allowables. This is carried out using the NSGA-II algorithm [38] to obtain a candidate set of process parameters expected to yield an excellently performing material, that should be tested next.

2 Formal process model

To efficiently capture and link all relevant data with their respective meta-data along the development process, the "flowthing" approach from [16] is adapted to the MDP. Specifying the "flowthing" in this context, the final material as well as its precursors are collected under the term material object (MO). Each MO is characterized by its features (Fs) and labeled with a unique identifier (UID). In PSs, the MO's Fs are changed, based on the present process parameters (PPs). The succession of multiple PSs that lead to a finished material are represented by a DAG, with the PSs characterized by a concrete set of PPs as its nodes and the MO being passed along its edges. The resulting heterogeneous graph constitutes one material manufacturing process (MMP). All MMPs that are carried out until design goal is met, combined with the reasoning behind respective changes of PPs across different MMPs, comprise the MDP. The formalized relationships are illustrated in Fig. 1.

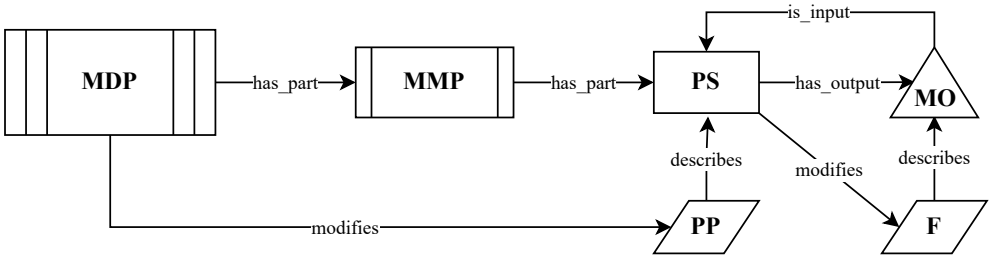


Fig. 1 Relationships of material development process and its constituents

The formal relationships lay the foundation for a general database scheme capable of storing data from diverse processes and sources. To ensure a lean database, it is possible to reduce the tracked PPs in this step based on expert knowledge on the process on hand.

From the proposed formalism, three approaches for establishing a surrogate model of the process of interest can be followed:

1. A PS based one, in which the property changes caused by each PS are modeled explicitly and are propagated to the next PS. This allows the targeted use of models for individual PSs, where existing knowledge can be incorporated directly. However, this requires information on the current state of Fs after each PS, imposing an enormous testing effort on the MDP.
2. A black box solution that aggregates PPs along the edges of the graph and correlates them with the final Fs. This requires the least amount of tests per MMP, but significantly hinders the possibility of including expert knowledge into the process model.
3. A hybrid solution between 1. and 2., in which relevant Fs are determined based on preexisting knowledge after steps that significantly influence them. This allows for the abstraction of multiple PSs into one, enabling a usecase specific trade-off between modeling fidelity and efficiency.

Having such a surrogate model allows to quickly estimate how changes to the process will influence the resulting product. This can be used for inline process monitoring to check if deviations from the intended PPs will be detrimental to the final Fs. Additionally, such a model may be used for accelerating the MDP by black box optimization. The model's sequential evaluation with PPs obtained from established optimization frameworks allows to quickly converge to an arbitrary objective or assess the pareto frontier when multiple objectives have to be considered.

3 Investigation of the applicability to a real world MDP of HMS

In this work, a manufacturing process for Fe-Ti-B-Cu HMS adapted from [39] is used as example. Instead of liquid metallurgy and casting, a powder metallurgical approach in combination with a hot isostatic pressing (HIP) process for the creation of ceramic TiB_2 particles is followed, as suggested in [40]. The final material is obtained by HIP and subsequent heat treatment. For the HMS, physical properties Young's modulus E and density ϱ, as well as mechanical properties yield strength (YS), ultimate tensile strength (UTS) and total elongation (TE) are of interest.

3.1 Building up graph representation of the MMPs

The powder production consists of the PSs `melting`, `atomization` and `sieving` . The `HIP` process is considered an atomic PS. The final product is obtained by heat treatment, consisting of `hardening` and `aging`. This leads to the graph representation shown in Fig. 2.

For the further analyses, powder production is not taken into account, since no data is available for the PPs of the PS `melting`, `atomization` and `sieving`.

3.2 Surrogate modeling of the MDP

Given the lack of data on changes in Fs throughout each MMP, a black box approach is chosen for the surrogate models. Hence, for each MMP all PPs are accumulated along the edges of the DAG and jointly correlated with the corresponding F obtained

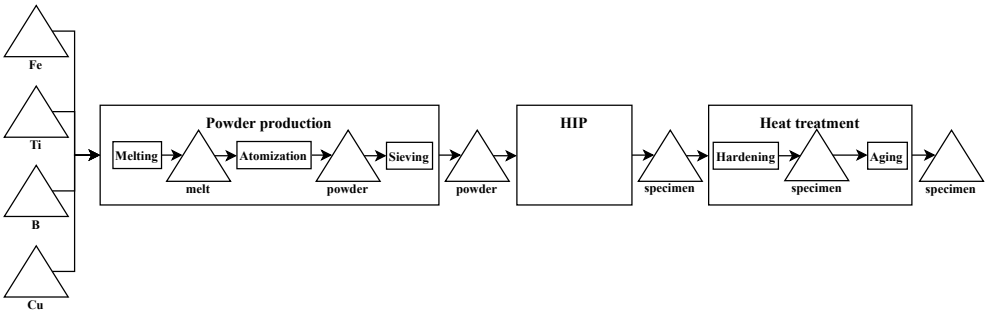


Fig. 2 Graph representation of an MMP for HMS

from the final MO. A total of 4 different chemical compositions were manufactured. These were subjected to different HIP and heat treatment conditions, leading to a total of 22 unique datapoints the MDP, which will be used for training the surrogate models. However, the physical properties are expected to be purely dependent on the chemical composition. Hence, only 4 experimental datapoints exist for these Fs. To alleviate the lack of data for the physical properties, for E 25 datapoints obtained from simulation[1] and for ϱ the 14 datapoints from literature given in Tab. A1 are added.

Based on the available data, several surrogate models are investigated for predicting individual Fs from chemical composition and PPs. Here, the following models from the open source Python library scikit-learn [41] are compared: 1. linear model, 2. stochastic gradient descent (SGD), 3. support vector regression (SVR), 4. GP and 5. multilayer perceptron (MLP). For each of them, except for the linear model, hyperparameter optimization (HPO) is carried out using the hyperopt library [42]. To do this, 15 % of the available data is withheld from training and used for validation. As an objective function for HPO, the RMSE on the validation set is used. The resulting contamination of the validation data has to be accepted, since the available data is too sparse to allow for a separate test set. The RMSE normalized by the respective means of the Fs is shown in Fig. 3 for each model.

From this it becomes clear, that different models are better suited for different Fs. Especially for the physical properties, SGD performs significantly worse than the other models. For the mechanical properties, models show very similar performance. For the final analyses, the best-in-class model for each F is chosen based on the lowest RMSE: 1. SVR for E, 2. GP for ϱ, 3. linear for YS, 4. linear for UTS and 5. SVR for TE. The corresponding hyperparameters are shown in Tab. 1 along with the achieved RMSE values.

For these best-in-class models, the comparison of actual and predicted values is shown in Fig. 4 on normalized values. From this it becomes clear that the models show overall very good performance. Especially for E, the SVR model excellently captures the behavior of the data, seamlessly integrating the simulation data. With ϱ, the GP model gives accurate predictions in spite of the literature data partly deviating from the simplifying assumption of a pure dependency on the chemical composition. The

[1] Simulations were carried out by QuesTek Innovations LLC.

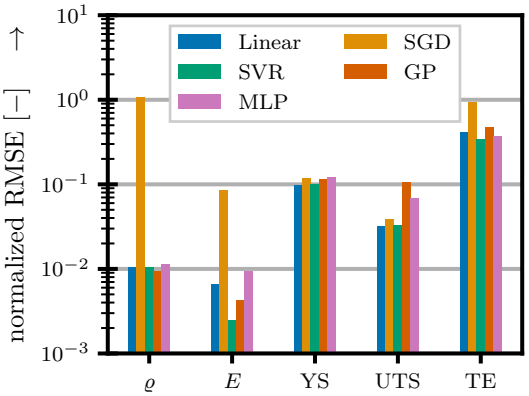


Fig. 3 Comparison of the normalized RMSE obtained from investigated surrogate models evaluated on validation data

Table 1 Hyperparameters and RMSE for the best-in-class surrogate models

Property	Model	Hyperparameters	Train RMSE	Train r^2	Test RMSE	Test r^2
E	SVR	C 54.835 epsilon 0.2974 degree 5 kernel "RBF"	0.0198	0.95	0.0025	0.99
ϱ	GP	kernel "RationalQuadratic" alpha 1 length_scale 1	0.0109	0.70	0.0093	0.76
YS	Linear	–	0.1300	0.59	0.0983	0.70
UTS	Linear	–	0.0472	0.83	0.0324	0.82
TE	SVR	C 12.241 epsilon 0.1011 degree 4 kernel "Linear"	0.2378	0.59	0.3436	0.40

more complex strength based mechanical properties are also well captured by the models. For the YS, an r^2 score of 0.70 is achieved on the test set using the linear model. Similarly, the UTS is predicted with an r^2 score of 0.82. Solely for the TE, the SVR model shows a lower performance, with an r^2 score of 0.40. This can be attributed to the high variability of the data in combination with the comparatively low number of datapoints available for training.

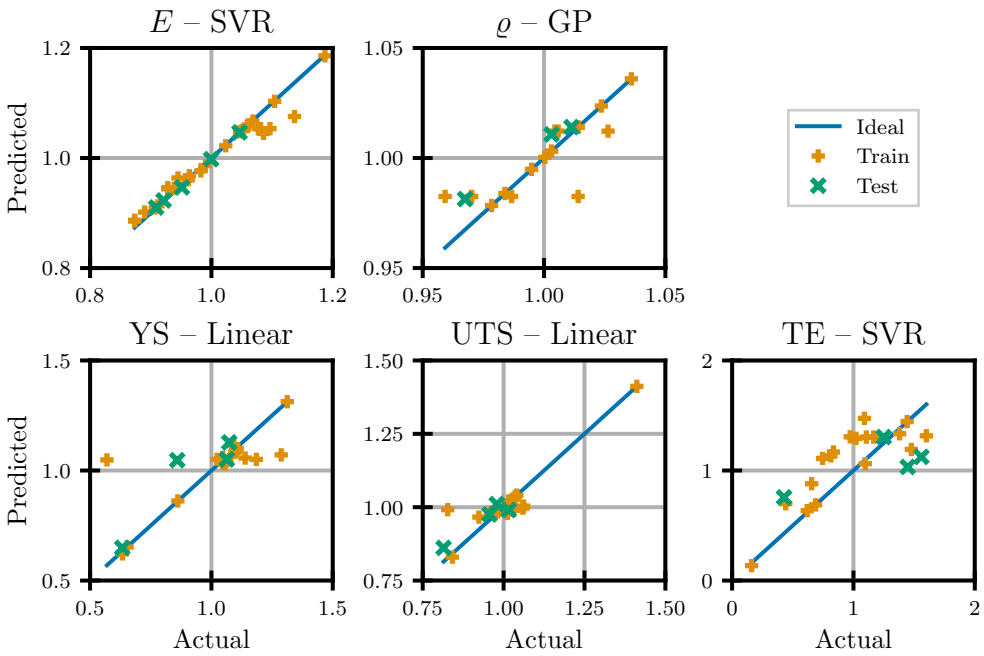


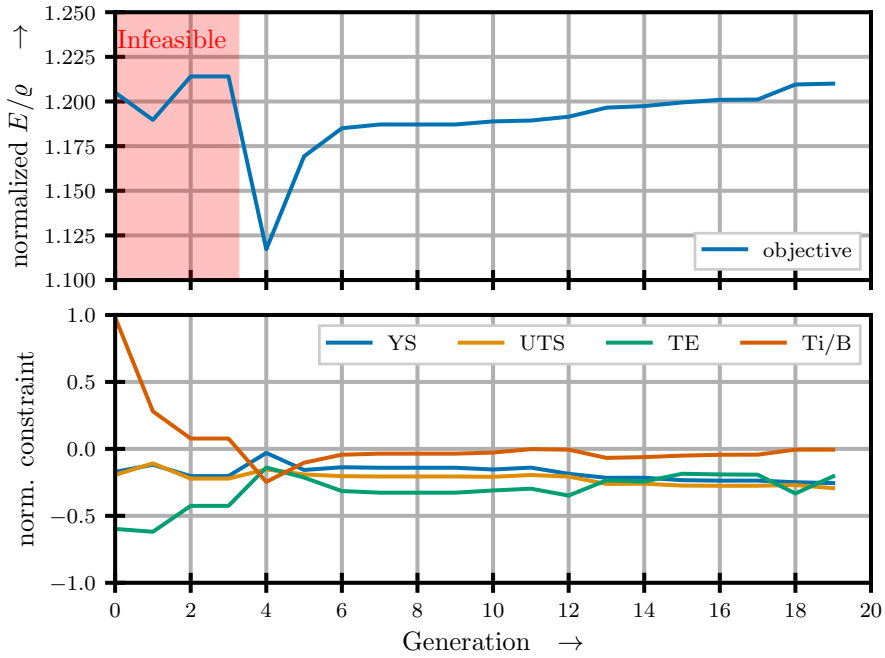
Fig. 4 Comparison of actual and predicted values for the best-in-class HMS surrogate models on normalized values

3.3 Extraction optimal PP to maximize specific modulus of the HMS

To optimize the material's performance without additional experimental effort, the determined models are used. Based on them, the target of maximizing specific modulus, an objective is defined per $\mathcal{O} = {}^{E}/_{\varrho}$.

This problem statement is implemented as `ElementwiseProblem` using the open source python library pymoo . The actual optimization is carried out using the NSGA-II algorithm with a population size of 40 and 20 generations. The normalized results are shown in Fig. 5.

From this it becomes clear that initially, a very high specific modulus is predicted. However, this is achieved with a chemical composition leading to an undesirable microstructure. Throughout the optimization a viable candidate is quickly identified in generation 4, at a high cost of the objective. From that point forward, slight modifications to the candidates lead to a gradual improvement of the objective function whilst remaining at the verge of the feasible region of the chemical composition. Throughout the optimization, in each generation candidates not violating the constraints on mechanical properties are achieved. Based on this, a combination of chemical composition and PPs is identified, that is predicted to have on par specific modulus with the best tested results, while meeting all design constraints.



In addition to that, several constraints from the design process have to be considered: for functionality, all mechanical properties have to exceed a certain threshold and to ensure the desired microstructure, the ratio of Ti and B has to be in a defined range.

Fig. 5 Results from optimizing chemical composition and PP for maximum specific modulus

4 Conclusion

To model MDPs and enhance them by data driven guidance, two established concepts for general process modeling were combined: 1. graph based representation of processes and 2. attaching information to an object that is passed along the process. This gave rise to a formalism for representing MDPs, which allows to efficiently derive a DAG representation. The functionality has been shown exemplary on the MDP of an HMS. Based on the derived DAG and available Fs, a database for subsequent training of surrogate models was established. This database was extended using data from simulations and literature for the physical properties, since the assumption of them being only influenced by the chemical composition lead to a severe reduction in available data.

Based on the database, a multitude of black box models for each F were trained, each representing one entire MMP. To obtain the best possible model, during this stage HPO was carried out for each investigated model type. From those the best-in-class model was chosen based on the RMSE on the test set for each F respectively. The models showed good performance for all properties except the TE. Using the established models, a candidate of chemical composition and PPs was identified that is predicted to lead to a significant improvement of the specific Young's modulus

while meeting all design targets on the mechanical properties and ensures a favorable microstructure. This should be the next point in the sequential design.

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Acronyms.

ANN	artificial neural network
BPMN	business process model and notation
DAG	directed acyclic graph
DOE	design of experiment
DSM	design structure matrix
F	feature
GP	Gaussian process
HIP	hot isostatic pressing
HMS	high modulus steel
HPO	hyperparameter optimization
MDP	material development process
MLP	multilayer perceptron
MMP	material manufacturing process
MO	material object
PP	process parameter
PS	process step
RMSE	root mean squared error
SGD	stochastic gradient descent
SLM	selective laser melting
SPH	smooth particle hydrodynamics
SVR	support vector regression
TE	total elongation
UID	unique identifier
UTS	ultimate tensile strength
YS	yield strength

Declarations

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Conflict of interest

The authors have no conflicts of interest to declare that are relevant to the content of this article.

Ethics approval and consent to participate

Not applicable.

Consent for publication

All authors have read the manuscript and agree with its publication.

Data availability

Materials availability

Code availability

Author contribution

Johannes Gerritzen: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Data Curation, Writing - Original Draft, Writing - Review & Editing, Visualization, Funding acquisition; **Andreas Hornig**: Resources, Writing - Review & Editing, Supervision, Project administration, Funding acquisition; **Maik Gude**: Writing - Review & Editing, Supervision, Project administration, Funding acquisition

Appendix A Enrichment of dataset

Table A1 Density values for HMS added from literature

Alloy-system	density in g/cm^3	Reference
Fe–13 TiB_2–3.7 Fe_2B	7.32	[43]
Fe–12.8 TiB_2–5.1 Fe_2B	7.32	[43]
Fe–13 TiB_2–7.9 Fe_2B	7.3	[43]
Fe–11.5 B–5.1 Ti	7.40	[7]
Fe–10.5 B–5.2 Cr	7.59	[7]
Fe–4.61 Ti–1.78 B	7.56	[44]
Fe–10.10 Ti–3.86 B	7.08	[44]
Fe–10.10 Ti–3.86 B (20 % TiB_2)	7.2	[45]
Fe–10.10 Ti–3.86 B (24 % TiB_2)	7.0	[45]
Fe–10.10 Ti–3.86 B (12 % TiB_2)	7.4	[45]
Fe–6.38 Ti–2.4 B	7.38	[46]
Fe–6.38 Ti–2.4 B	7.4	[46]
Fe–9.43 Ti–3.74 B	7.06	[39]
Fe–10.7 Ti–3.74 B–1.07 Cu	7.26	[39]
Fe–9.32 Ti–3.12 B–2.07 Cu	7.47	[39]
Fe–1.6 B–18.8 Cr	7.54	[47]
Fe–18.8 Cr–1.6 B–1 Cu	7.40	[47]
Fe–1.80 B–24.0 Cr	7.43	[48]

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