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Editorial

Artificial Intelligence for Crystal Growth and Characterization

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The Special Issue on "Artificial Intelligence for Crystal Growth and Characterization" comprises six original articles in this emerging field of research. AI methods have already found relatively wide exemplary applications in materials science in general, where they have triggered major efforts to establish common data infrastructures ranging from within individual organizations to the national level (e.g., the National Research Data Infrastructure for Materials Science & Engineering NFDI MatWerk in Germany, or as part of the Materials Genome Initiative in the US). The so-called FAIR (findable, accessible, interoperable, and reusable) data infrastructures are currently under development in order to serve as an enabling infrastructure for AI-assisted research [1]. International data infrastructures appear to be contemplated, albeit at a very early stage, as there are still many challenges to be resolved even at much smaller organizational levels. Such challenges include the standardization of nomenclature and experimental procedures. Inherent to the challenge of establishing data infrastructures and best practices is also an educational challenge, as these tasks demand expertise in AI methods and informatics as well as solid domain knowledge.

One contribution from the area of crystal structure prediction investigates the possible bulk Cr–Si–N phases of the composition of Cr_2SiN_4 via a cross-methodical approach combining global optimization, data mining, and the Primitive Cell approach for Atom Exchange (PACE) [2]. In the field of the plastic deformation of polycrystalline materials, the use of knowledge graphs representing microstructures is explored for predicting the twin density of materials subjected to specific tensile deformation [3]. The application of AI methods to subdisciplines with smaller numbers of data, such as bulk crystal growth, is only nascent. Nevertheless, four articles in this Special Issue have addressed the growth of semiconductor materials as bulk crystals or thin films [4–7]. Two of them target the growth of GaAs via the Vertical-Gradient-Freeze (VGF) method [4,5]. The successful application of recurrent Long Short-Term Memory (LSTM) neural networks for fast and accurate predictions of process dynamics, including temperatures and the position of the solid–liquid interface, was realized using a dataset of transient numerical simulations [4]. The other contribution on VGF growth of GaAs evaluates the capabilities of various data-mining and supervised machine-learning techniques for identifying and optimizing the key factors that influence the growth process [5]. One contribution from the field of studying the ammonothermal growth of GaN applied machine learning for parameter selection in the numerical simulation of a growth setup with varying heater powers [6]. In the field of the thin film growth of β-Ga_2O_3 via metalorganic vapor epitaxy (MOVPE), doping with Si has been investigated using a hybrid deep-learning model (fDNN, Forest Deep Neural Network) for predicting the doping level obtained from the Hall measurements [7]. This led to the identification of the Si supplied per nanometer (mol/nm) as a hidden parameter of previously unrecognized relevance [7].

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Citation: Schimmel, S.; Sun, W.; Dropka, N. Artificial Intelligence for Crystal Growth and Characterization. *Crystals* **2022**, *12*, 1232. https://doi.org/10.3390/cryst12091232

Received: 26 August 2022
Accepted: 29 August 2022
Published: 1 September 2022

It is evident that the data generated by numerical simulations currently play a major role in the exploration of AI applications in the field of bulk crystal growth. This particularly applies to research at public institutions such as universities and research institutes, which usually engage in the early stages of development rather than the scale-up and large-scale optimization and often do not have the resources to produce large experimental datasets in research areas where the cost of a single experiment is high. Especially in bulk crystal growth, the cost of experiments is often dominated by investment costs in crystal growth reactors, extended process durations, and certain consumables. Contrary to some other fields of material synthesis, the cost of experimental data generation for bulk crystal growth cannot be decreased by automation to the same degree. Consequently, the attempts of applying AI methods with the use of large experimental datasets appear mostly in industrial crystal growth, where larger amounts of data of a single type of growth process are naturally generated, partially as a byproduct of production or in pilot plants. For methodical developments as well as for the education of next-generation crystal growth researchers, two areas of action shall be highlighted. Firstly, hybrid approaches that integrate physical knowledge into AI models deserve further attention, as this process can significantly reduce the degrees of freedom and may facilitate the successful use of adapted AI methods with small to medium sized datasets. However, such hybrid approaches require the combination of domain knowledge and the ability to not only apply existing general AI methods but also to develop and adapt them to the respective problem. Therefore, the bidirectional mobility of people between disciplines engaging in crystal growth and characterization (e.g., materials science, physics, chemical engineering, and chemistry) and informatics should be encouraged. Secondly, for the educational and methodical developments in the use of comparatively large datasets, the mobility of either people or data between public and private institutions needs to be fostered. This may take the form of academia–industry collaboration as well as, prospectively, the development of adapted strategies and platforms for the responsible joint use of selected data.

Considering that there is still no general theory describing crystal growth processes due to their multidisciplinary nature, high complexity, and the different length scales and time scales involved, it can be expected that AI will also significantly accelerate basic research in the future. Applying data-driven approaches to synthesis science represents a 'top-down' perspective, where machine-learning algorithms aim to identify trends and correlations in large swaths of empirical data. On the other hand, the traditional 'bottom-up' approach of physics-driven derivation is still important, and its most important deliverables are conceptual guidance and scientific intuition. Thus, the challenges and opportunities should involve developing synergies to meet in the middle, such that AI can enable us to take advantage of big datasets, while also building new physical and conceptual insights that we can teach ourselves and other scientists. Using the time- and cost-efficient predictive power of AI, new kinetic and thermodynamic crystal-growth theories will be validated and compared to existing ones. From this perspective, AI methods can be understood as valuable partners to the scientist for the development of a general crystal-growth theory.

In conclusion, the application of AI methods in the field of crystal growth has just begun. Some promising first applications have been demonstrated and are being developed. While the general tools of AI are now easily available and have already significantly lowered the entry barriers, the current bottlenecks lie in the experience and methodical knowledge of domain experts, data infrastructure and standardization, and the amount and availability of data.

Ongoing developments regarding data infrastructure for materials science can be expected to catalyze further developments in more specialized subdisciplines such as crystal growth and characterization. The articles in this Special Issue will hopefully inspire further activities in the crystal growth community.

Funding: The initiating guest editor (S.S.) is grateful for the financial support of the Japan Society for the Promotion of Science (Postdoctoral Fellowships for Research in Japan (Standard), grant number P19752) and the Alexander von Humboldt-Foundation (Feodor Lynen Return Fellowship) that has contributed to the realization of this Special Issue through funding of the initiating guest editor's research activities.

Acknowledgments: The guest editors thank all authors for their contributions and the Editorial Office for supporting this Special Issue.

Conflicts of Interest: The authors declare no conflict of interest.

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