Data-driven Cz-Si scale-up under conditions of partial similarity

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Scale-up is a process of moving from small scale to commercial facilities, ensuring that the two systems remain physically similar and that the small-scale results can then be transferred to the large-scale without limitations. This can be achieved by applying a similitude principle [1], which consists in keeping the dimensionless numbers characterizing the transport phenomena constant during upscaling. These numbers or their combinations (e.g. $1/Re \cdot Pr$, $1/Re \cdot Sc$, Gr/Re^2, etc.) come from dimensionless form of governing conservation equations for the transport phenomena taking place during crystal growth.

To achieve similitude between crystal growth processes on two scales, all criteria must be met: geometric, kinematic, dynamic and thermal similarity. In complex processes such as Cz-Si growth, the similarity rules are challenging as some conditions may be contradictory, material properties may be difficult to find in real materials when model materials have been used before at the small scale (e.g. salts vs. Si), different phenomena can be difficult to distinguish from each other (e.g. melt flow generated by crystal rotation vs. by crucible rotation), geometry is only similar to a certain extent (e.g. relative position, material properties, shape and aspect ratio of heaters, heating shields and crucibles may vary). The following methodology is proposed in [2-4] for examining the cases with partial similarity [2] in chemical engineering applications: i) the processes are broken down into individual parts, which are then examined separately, ii) certain similarity criteria are deliberately abandoned and the subsequent effects on the overall process are checked, or iii) characteristic variables are defined differently.

The aim of this study was to investigate the scale up under partial similarity conditions and the consequences of such an approach using the Cz-Si growth as a case study. The Cz-Si was chosen for its importance in modern electronics and high-performance photovoltaics where upscaling ingot size with very high scale ratios is still a challenge. It is also a slow process, i.e. it took 40 years to increase the Si crystal diameter from 1 inch to 12 inches.

The complex nonlinear relationship between the crystal growth process parameters, the set-up geometry, the s/l interface shape, melt stream function and the thermal gradients in the melt and crystal was derived using artificial neural networks (ANN). The ANN approach was chosen due to its predictive accuracy and generalization ability as shown in [5]. The numeric training datasets were generated by axisymmetric CFD simulations for the Si ingot sizes from 4 to 18 inches and the loads from 5 to 450 kg.

Reference

[1] Kline SJ. *Similitude and Approximation Theory* (Springer-Verlag, NewYork. 1986).
[2] Zlokarnik M. Modellubertragung bei partieller Ahnlichkeit, Chem.-1ng.-Tech. 1985;57: 410-416.
[3] Froude W. On experiments with H.M.S. “Greyhound”. Trans. Inst. Naval Arch. 1874; 15: 36-73.
[4] Damköhler G. Einflüsse der Strömung, Diffusion und des Wärmeüberganges auf die Leistung von Reaktionsöfen.: I. Allgemeine Gesichtspunkte für die Übertragung eines chemischen Prozesses aus dem Kleinen ins Große. Z. Elektrochem. 1936; 42: 846-862.
[5] Dropka N and Holena M. Application of Artificial Neural Networks in Crystal Growth of Electronic and Opto-Electronic Materials. Crystals. 2020; 10: 00663.