

Program of Session C

Advances in Modelling Crystal Growth Processes Including AI

C1: August 4 (Monday), 14:00-15:40

Room: 210

Chair: Zheng, Lili, Stanialaw Krukowski

14:00-14:25

C01 (Oral)

Data science of the in silico crystallization

Redkov Alexey ^{*1}, Trotsenko Danil²

1. Institute for Problems in Mechanical Engineering RAS, RUSSIA

2. National Research University ITMO, RUSSIA

14:25-14:50

C02 (Oral)

A Neural-Network surrogate for microstructure dynamics and crystal growth

Daniele Lanzoni, Andrea Fantasia¹, Matteo Rigoni, Francesco Montalenti, Roberto Bergamaschini^{*},

University of Milano-Bicocca, ITALY

14:50-15:15

C03 (Oral)

Understanding Native Defects in GaN Under MOCVD Conditions: A Computational Perspective

Roman Hrytsak^{*1}, Pawel Kempisty¹, František Hájek², Jakub Čížek³, Ewa Grzanka¹, Robert Czernecki¹, Mike Leszczynski¹

1. Institute of High Pressure Physics, Poland Academy of Sciences, POLAND,

2. Institute of Physics (Czech Academy of Sciences), CZECH REPUBLIC

3. Charles University, CZECH REPUBLIC

15:15-15:40

C04 (Oral)

Configurational entropy in solid and liquid silicon

Jinping Luo^{*1}, Lijun Liu¹, Jack F. Douglas², Talid Sinno³,

1. School of Energy and Power Engineering, Xi'an Jiaotong University, CHINA

2. Material Measurement Laboratory, Material Science and Engineering Division, National Institute of Standards and Technology, Gaithersburg, USA

3. Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, USA

C2: August 4 (Monday), 16:00-17:15

Room: 210

Chair: Zheng, Lili, Dropka, Natascha

16:00-16:25 **C05 (Oral)**
Are Commercial Simulation Tools Advancing or Hindering Crystal Growth Modeling?
Chung wen Lan,
National Taiwan University, CHINESE TAIBEI

16:25-16:50 **C06 (Oral)**
Determination of Cracking Criteria and Crack-free Control Strategies for Doped BaF₂ Crystals Growth by Bridgman Technique
Jiahe Li¹, LiLi Zheng^{*1}, Hui Zhang¹, Jing Zhang², Junfeng Chen²
1. Tsinghua University, CHINA
2. Shanghai Institute of Ceramics, CAS, CHINA

16:50-17:15 **C07 (Oral)**
Numerical Simulation of Coupled Internal Thermal Radiation and Anisotropic Thermal Conduction in β -Ga₂O₃ Crystal Growth by EFG
Wang Junlan, Li Zaoyang*, Liu Lijun
Xi'an Jiaotong University, CHINA

C3: August 5 (Tuesday), 11:00-12:40

Room: 210

Chair: Dropka, Natascha; Liu, Lijun

11:00-11:25 **C08 (Oral)**
Effects of segregation of impurity on temperature and dislocation density distributions in a crystal and the melt of β -Ga₂O₃ grown by the VB method
Koichi Kakimoto^{*1}, Taketoshi Tomida², Vladimir V. Kochurikhin², Kei Kamada^{1,2}, Satoshi Nakano³, Akira Yoshikawa⁴
1. Tohoku University, JAPAN
2.C&A Co. , JAPAN
3.Kyushu University, JAPAN
4.Tohoku University, JAPAN

11:25-11:50 **C09 (Oral)**
Numerical Simulation of Impurities and Defects in n-Type 4H Silicon Carbide
Xuefeng Han*, Lingling Xuan, Anqi Wang, Sheng'ou Lu, Xiaodong Pi, Deren Yang,
Zhejiang University, CHINA

11:50-12:15 **C10 (Oral)**
Stability-based optimization of ACRT for the growth of CZT by THM
Jeffrey H. Peterson, Zachary Cosenza, Jeffrey J. Derby*
University of Minnesota, USA

12:15-12:40 **C11 (Oral)**
Effects of crucible etching and polycrystal deposition in the top-seeded solution growth of SiC single crystal
Xiying Zhang, Wancheng Yu*, Xiufang Chen, Xiaobo Hu, Xiangang Xu
Shandong University, CHINA

C4: August 5 (Tuesday), 14:00-15:40

Room: 210

Chair: Liu, Lijun; Dropka, Natascha

14:00-14:25	<p>C12 (Oral) Control of 6H-SiC polytype inclusion for 4H-SiC single crystal growth by PVT method Jiazheng Lu¹, Lili Zheng^{*1}, Hui Zhang¹, Runguang Hu², Dongli Hu² 1. Tsinghua University, CHINA 2. Linko Advanced Technologies Co. Ltd., CHINA</p>
14:25-14:50	<p>C13 (Oral) Machine learning assisted design of SiC crystal growth based on the PVT method Lorenz Romaner, Lorenz Taucher, Zaher Ramadan Montanuniversität Leoben, AUSTRIA</p>
14:50-15:15	<p>C14 (Oral) SMART Growth: Artificial intelligence enhanced, sustainable growth of rare-earth materials-based laser crystals Philippe Veber^{*1}, Dragos Tatomirescu¹, Alexandra Popescu¹, Gabriel Buse¹, Daniel Vizman¹, Natasha Dropka² 1. West University of Timisoara, ROMANIA 2. Leibniz Institute for Crystal Growth, GERMANY</p>
15:15-15:40	<p>C15 (Oral) Insights from 3D Modeling of SiC Solution Growth: Unidirectional Solution Flow Realization by Asymmetric Hot-zone Designs Xin Liu[*], Tomoaki Furusho, and Toru Ujihara Nagoya University, JAPAN</p>

C5: August 5 (Tuesday), 16:00-17:15

Room: 210

Chair: Stanialaw Krukowski, Liu, Lijun

16:00-16:25	<p>C16 (Oral) Towards a Universal Czochralski Growth Model Leveraging Data-Driven Techniques Natasha Dropka^{*1}, Christiane Frank-Rotsch¹ and Martin Holena^{2,3} 1. Leibniz-Institut für Kristallzüchtung, GERMANY 2. Leibniz Institute for Catalysis, GERMANY 3. Institute of Computer Science, CZECH REPUBLIC</p>
16:25-16:50	<p>C17 (Oral) Machine Learning-Based Diameter Prediction and Critical Parameter Identification in CCZ-Si Chenyun Pan, Xuefeng Han[*], Lei Liu, Limin Jiang, Shuai Yuan, Deren Yang Zhejiang University, CHINA</p>
16:50-17:15	<p>C18 (Oral) A Kinetic Monte Carlo and Deep Learning Integrated Approach for Crystal Epitaxial Growth Simulation and Closed-Loop Control Ai Wensen^{*1}, Chen Xuejiang² 1. Chang'an University, CHINA 2. Xi'an Jiaotong University, CHINA</p>