ISMCG 1
THE 1ST INTERNATIONAL SCHOOL ON MODELING IN CRYSTAL GROWTH

1st INTERNATIONAL SCHOOL ON MODELLING IN CRYSTAL GROWTH
Timisoara, 19-21 September 2024

International School on Modeling in Crystal Growth is an accompanying event of the International Workshop on Modelling in Crystal Growth.
The School program includes lectures on theoretical, mathematical and practical aspects of the macro-simulation of crystal growth processes. Around this central theme, it will also propose introductions to complementary modeling techniques, at the atomic, microscopic and mesoscopic scales.

While mornings will be devoted to conventional lectures, afternoons will propose "on the screen" practical activities with 1) an in-depth case study of optimization of a bulk crystal growth process and 2) parallel workshops, animated by the lecturers, to familiarize with techniques such as DFT, Monte-Carlo, Phase Field or Artificial Intelligence.

The ISMCG1 will be organized at the West University of Timisoara, placed close to the city center. The university offers comfortable rooms for lectures and computer rooms for practical activities.

Co-chairmans of the ISMCG 1:
Thierry Duffar, SIMaP-EPM, France:
Daniel Vizman, West University of Timisoara

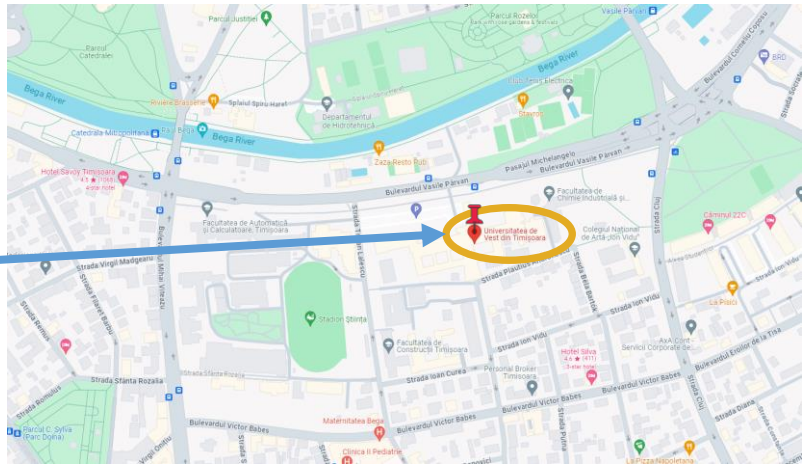
Lecturers who accepted participation in the school
Roberto Bergamaschini, University of Milano-Bicocca, Italy
Kaspars Dadzis, Leibniz Institute for Crystal Growth, Germany
Jeffrey J. Derby, University of Minnesota, USA
Thierry Duffar, SIMaP-EPM, France
Simon Brandon, Technion Institute of Technology, Israel
Marc Hainke, , Fraunhofer-Institute IISB, Germany
Kentaro Kutsukake, RIKEN, Japan
Lijun Liu, Xi'an Jiaotong University, China
Mathis Plapp, Ecole Polytechnique, France
Talid Sinno, University of Pennsylvania, USA

Website: https://iwmcg-11.uvt.ro/
Contact: iwmcg11@e-uvt.ro

Location

West University of Timisoara, Faculty of Physics

Bd. Vasile Parvan 4, Timisoara



Lectures: “Constantin Salceanu” amphitheater, 2½ floor Faculty of Physics

Practical activities: Rooms F202 A and F202 B, 2½ floor Faculty of Physics

Organized by:

International Organization for Crystal Growth

West University of Timișoara

The Romanian Physical Society

ISMCG-1 Program:

Thursday, September 19th 2024

08:00 – 08:30	Registration
8:30 – 9:00	Lecture 1 **Introduction** Various scales and technics for modelling crystal growth. Contents, organization and schedule of the school. **Thierry Duffar** *University Grenoble Alpes/Grenoble INP, CNRS, SIMAP, Grenoble, France*
9:00 – 10:00	Lecture 2 **Economical aspects** Several industrial examples on how modeling can help. Costs and benefits. **Marc Hainke**[1, 2] [1] *Fraunhofer IISB, Erlangen, Germany* [2] *Ostbayerische Technische Hochschule (OTH) Amberg-Weiden, Weiden, Germany*
10:00 – 10:20	**Coffee break**
10:20 – 11:50	Lecture 3 **Macro 1: Physical phenomena** Transport equations to be modeled (incl. magnetic field, dislocations, point defects …) **Jeffrey J. Derby** *Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis,U.S.A.*
11:50 – 12:10	**Coffee break**
12:10 – 13:40	Lecture 4 **Macro 2: Resolution techniques** How it works (Mesh, Matrix, Gauss, Newton, implicit/explicit …), FEM, FVM, view factors, impact of numerical parameters … **Simon Brandon** *Technion – Israel Institute of Technology, Haifa, Israel*

13:40 – 15:00	**Lunch break**
15:00 – 18:30	Practical session 1 **PRACTICAL 1 : CGSim** Building a model: Czochralski growth of Si crystal Playing with the numerical parameters (mesh, Δt, accuracy…) and some process effects (counter/co rotation …) **Andrey Smirnov** *Semiconductor Technology Research d.o.o. Beograd, Belgrade, Serbia*

Friday, September 20th 2024

8:30 – 10:00	Lecture 5 **Macro 3: The model** Various available codes, How to build a model, Validation of the model with experiments, Sensibility to physical parameters. **Kaspars Dadzis** *Leibniz-Institut für Kristallzüchtung (IKZ), Berlin, Germany*
10:00 – 10:20	**Coffee break**
10:20 – 11:50	Lecture 6 **Models for physico-chemical properties** Molecular behaviours (Monte Carlo, Molecular Dynamics…) **Talid Sinno** *Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, USA*
11:50 – 12:10	**Coffee break**
12:10 – 13:40	Lecture 7 **Simulation for epitaxial processes** Atomistic/molecular models for growth, Kinetic Monte Carlo … **Roberto Bergamaschini** *L-NESS and Dept. of Materials Science, University of Milano-Bicocca, Milano, Italy*
13:40 – 15:00	**Lunch break**
15:00 – 18:00	Practical session 2

	PRACTICAL 2 : CGSim Optimizing the Cz-Si model, Change geometry, physical parameters … to decrease interface deflection, stresses … comparison to experiment **Andrey Smirnov** *Semiconductor Technology Research d.o.o. Beograd, Belgrade, Serbia*
18:00 – 19:00	**POSTER SESSION**

Saturday, September 21th 2024

8:30 – 10:00	Lecture 8 **Macro 4: Case study** Industrial development of crystal growth technology based on crystal growth modeling **Lijun Liu** *Xi'an Jiaotong University, China*
10:00 – 10:20	**Coffee break**
10:20 – 11:50	Lecture 9 **Phase field** How it works. What can and cannot be expected. **Mathis Plapp** *Laboratoire de Physique de la Matière Condensée, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, Palaiseau, France*
11:50 – 12:10	**Coffee break**
12:10 – 13:40	Lecture 10 **Artificial Intelligence** Exemples of uses in crystal growth. How it works. **Kentaro Kutsukake**[1,2] [1]*Institute of Materials and Systems for Sustainability, Nagoya University, Nagoya, Japan* [2]*Graduate School of Engineering, Nagoya University, Nagoya, Japan*
13:40 – 15:00	**Lunch break**
15:00 – 18:30	Practical session 3 **PRACTICAL 3: parallel Workshops, 1.5 hours each** Groups of up to 5 students. Each group attends two workshops.

	- Phase field (Mathis Plapp) - AI-Neural network (Kentaro Kutsukake) - Monte Carlo for Epitaxy (Roberto Bergamaschini) - More CGSim (STR) - Elmer (Kaspars Dadzik) - Molecular Dynamics, short demo (Talid Sinno)
19:00 – 22:00	**School dinner**

Sunday, September 22th 2024

08:30 – 9:30	Lecture 11(Optional????) **Thermodynamics for Crystal Growth** Reminders, chemical reactions, phase diagrams, use of thermodynamic software and databases in the field of crystal growth **Thierry Duffar** *Université Grenoble Alpes/Grenoble INP, CNRS, SIMAP, Grenoble, France*
9:30 – 9:50	**Coffee break**
9:50-13:30	Practical session 4 (Optional????) **PRACTICAL 4: parallel Workshops, 1.5 hours each** Groups of up to 5 students. Each group attends two workshops. - Phase field (Mathis Plapp) - AI-Neural network (Kentaro Kutsukake) - Monte Carlo for Epitaxy (Roberto Bergamaschini) - More CGSim (STR) - Elmer (Kaspars Dadzik) - Molecular Dynamics, short demo (Talid Sinno)