FACET



DACG NEWSLETTER

September 2021 Issue 2

FACET

Newsletter of the Dutch
Association for Crystal Growth
(DACG), section of the KNCV and
the NNV.

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CONTENT:	PAGE:
FROM THE EDITOR, UPCOMING EVENTS	2
REPORT OF DACG SPRING SYMPOSIUM	3
DACG GOES TELEGRAM	4
AGENDA & REGISTRATION FOR ANNUAL	
MEETING AND FALL SYMPOSIUM	5
AGENDA FOR DACG ANNUAL MEETING 20	21 6
ANNUAL REPORT DACG 2020-2021	7
RECENT PUBLICATIONS & THESES	10



DACG Secretary

Prof.Dr. Antoine van der Heijden Leeghwaterstraat 39 2628 CB Delft

DACG board

Dr. Hans te Nijenhuis (Malvern Panalytical)	chairman
Prof.Dr. Antoine van der Heijden (TUD)	secretary
Dr. Pieter Vonk (DSM)	treasurer
Dr. Hugo Meekes (RU)	WWW
Dr. Marketta Uusi-Penttilä (Aspen Oss)	FACET

Cover figure

A photo of a "surface of lead carbonate nanocrystals that are converted into light-emitting perovskite crystals in the form of a portrait of Marie Curie (by Lukas Helmbrecht, Wim Noorduin, AMOLF, Amsterdam).

From the editor

Dear all,

I hope that you have had a relaxing summer.

The annual meeting 2021 and fall symposium will be held online on Friday October 8^{th} : The annual meeting 11:00-12:00, followed by "Meet the town" session over lunch and the fall symposium 13:00-15:00.

Due to postponement of several conferences and symposia, our 50th anniversary will take place in 2023 (50+1 years). Please do not hesitate to share your highlights of 50 years of crystal growth in the Netherlands, including pictures of your historical crystal growth or crystallization installations.

Your ideas are welcome, and as always, it is easy to contribute to the FACET. Just send an email to the editor: Marketta Uusi-Penttilä

Keep safe! Marketta Uusi-Penttilä

Upcoming events

- KNCV-event "Avond van de Chemie", 14 October 2021, Parktheater Eindhoven (https://www.kncv.nl/bijeenkomsten/922/avond-van-de-chemie-2021#.YSNdiXzivIU)
- DACG Annual Meeting, 8 Oct 2021 11:00-12:00, Online
- DACG Fall Meeting, 8 Oct 2021 13:00-15:00, Online
- DACG Spring Meeting, Apr 2022, tbd.



DACG Spring Symposium 2021

9 April 2021, online

On 9 April 2021, the DACG organized her first online spring symposium after more than a year during which no symposia were organized due to the COVID-19 measures. The online symposium was attended by 26 participants. Hans te Nijenhuis welcomed all participants and especially the five speakers that were invited to give a presentation on their research topics.

Simon Lepinay (UvA) was the first speaker, reporting on nature-inspired multi-mineral salts for iron fortification. **Ernest van der Wee** (TU Delft) continued with a presentation on his PhD research performed at the University of Utrecht on binary icosahedral clusters of hard spheres in spherical confinement.

During the coffee break, **Marloes Bistervels** (AMOLF) informed the audience about a new initiative for setting up a communication platform to stimulate contacts between the DACG members; this platform can also help in connecting expertise and experimental facilities available within different academic or industrial groups. Marloes requested the participants to fill out a survey to explore the requirements that the communication platform should fulfil.

After this break a presentation was given on growth of pure polytypes in GaAs nanowires by **Marco Vettori** (TU/e). Self-lifting NaCl crystals were discussed by **Herish Salim** (UvA) and finally **Francesc Valls Mascaró** (University of Leiden) presented his results on decreasing degradation of platinum which is used as a catalyst for fuel cell operation.

Although the online symposium was a success, we hope to be able to organize 'live' symposia again in the near future.







DACG goes Telegram!

Dear all,

My name is Marloes Bistervels, a PhD student of Wim Noorduin in the Self-Organizing Matter group at AMOLF (in Amsterdam). Together with the board of the DACG, I am investigating the connection of peers in this field.

Thank you to everyone that filled in the survey. This was super helpful. In summary, the survey was filled in by 17 people, ranging from PhD students, professors, and professionals in the industry. Responses were indicating that there is interest for more contact with peers and a central point of information. However, from the survey, it was also clear that many already are occupied with a lot of tasks and an additional communication platform can have the risk of overfeeding.

Therefore, I asked some PhD students and Post-docs from Wageningen, Eindhoven, and Amsterdam to further discuss our needs and preferences in communication. We concluded to start with something very small and rather informal: a telegram group for crystal growth-related topics!

In this telegram group, we can keep each other updated on publications, ask questions, ask for equipment, share an interesting event, or something else related to your work in crystal growth.



You can add yourself via the following link or scan the QR code: https://t.me/joinchat/9he5nEYTQbFiMDc0



Feel free to invite more colleagues that can benefit from this.

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Best,

Marloes



DACG Annual meeting 2021 & Fall Symposium

Online, 8 October 2021

11:00 - 12:00	Annual meeting (see agenda on next page) Hans te Nijenhuis
12:00 - 13:00	Lunch break / Gather.town
13:00 - 13:10	Welcome and introduction Hans te Nijenhuis
13:10 - 13.25	Young-DACG Marloes Bistervels (AMOLF)
13:25 - 13:50	In remembrance of Prof dr ir Gerda M. van Rosmalen Herman Kramer and Antoine van der Heijden (Delft University of Tech- nology)
13:50 - 14:15	Steering crystallization with light, flow and soft matter Burak Eral (Delft University of Technology)
14:15 - 14:25	Break
14:25 - 14:50	Towards effective crystallization by using small scale crystalliz- ers. 17 Years of Crystallization Carmen Guguta (Technobis)
14:50 - 15:00	Closing remarks Hans te Nijenhuis

Registration

To receive the MS Teams meeting invitation, please register by sending an email titled "Registration for DACG Fall Symposium" to

a.e.d.m.vanderheijden@tudelft.nl by 4 October 2021.



DACG Annual Meeting 2021

8 October 2021 11:00-12:00, online via MS Teams

- 1. Opening
- 2. Finalize agenda
- 3. Minutes Annual meeting 9 October 2020 (online)
- 4. Documents sent / received:
 - a. Report financial audit committee 2020
 - b. Report from the jury to select the prize winner of the KNCV Piet Bennema Crystal Growth Award 2021
- 5. Annual Report Oct 2020 Oct 2021
- 6. Financial
 - (a) Annual Report Oct 2020 Sep 2021
 - (b) Report Financial Audit Committee
 - (c) Budget 2021-2022
- 7. Board

Role	2020 – 2021	Appointment deadline
President	Hans te Nijenhuis	Step down Oct 2021
Secretariat	Antoine van der Heijden	Step down Oct 2022
Treasurer	Pieter Vonk	Step down Oct 2021 (not re-electable)
Webmaster	Hugo Meekes	Step down Oct 2023
FACET	Marketta Uusi-Penttilä	Step down Oct 2023

Two of the DACG board members step down. DACG-members who would like to apply for a board membership, can announce themselves by sending an e-mail to the DACG secretariat (a.e.d.m.vanderheijden@tudelft.nl), ultimately by 30 September 2021. At this moment one new candidate has registered.

- 8. 2021: KNCV Piet Bennema Crystal Growth Award
- 9. 2022: DACG 50 years
- 10. Status Stichting
- 11. Young-DACG (update by Marloes Bistervels)
- 12. Activities 2021 2022
 - a. KNCV-event "Avond van de Chemie", 14 October 2021, Parktheater Eindhoven (https://www.kncv.nl/bijeenkomsten/922/avond-van-de-chemie-2021#.YSNdiXzivIU)
 - b. NNV-adviesraadvergadering, December 2021 (section boards will be invited)
 - c. April 2022: DACG spring meeting, University of Utrecht, date to be decided
 - d. October 2022: Annual meeting + symposium, date/location to be announced
- 13. Questions before closure of meeting
- 14. Adjourn

Registration

To receive the MS Teams meeting invitation, please register by sending an email titled "Registration for DACG Annual Meeting" to

a.e.d.m.vanderheijden@tudelft.nl by 4 October 2021.



Annual Report Dutch Association for Crystal Growth (DACG) October 2020 – October 2021

Secretariat

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Members

The total number of regular members is 31. This year, due to COVID19, we did not organize "live" DACG meetings¹, so we did not have any additional "calendar year" members. Last year (2019-2020) we had 14 "calendar members", which are still offered the possibility to attend a DACG symposium for the registration fee of a regular DACG member, once a symposium can be organized again as a face-to-face meeting.

Board

The DACG Board is summarized in the table below. The Board had six online video meetings (due to COVID19 no face-to-face meetings).

Role	2020 – 2021	Appointment deadline	E-mail
President	Hans te Nijenhuis	Step down Oct 2021	hans.te.nijenhuis@panalytical.com
Secretary	Antoine van der Heijden	Step down Oct 2022	a.e.d.m.vanderheijden@tudelft.nl
Treasurer	Pieter Vonk	Step down Oct 2021	pieter.vonk@dsm.com
Webmaster	Hugo Meekes	Step down Oct 2023	h.meekes@science.ru.nl
FACET	Marketta Uusi-Penttilä	Step down Oct 2023	muusipenttila@nl.aspenpharma.com

FACET Newsletter

The DACG Newsletter, FACET, was issued in March and September 2021. Dr Marketta Uusi-Penttilä is the editor of the FACET. The objective of the newsletter is to stimulate the communication between scientists and users in the area of crystallization in the Netherlands. The newsletter publishes summaries of relevant PhD theses, upcoming events related to crystallization (conferences, symposia), highlights in crystal growth research and other activities relevant to crystal growers. Several academic scientists have been requested to collect news from their network/colleagues as input to the newsletter, but also members may submit input. Furthermore, initiatives, decisions and plans of the DACG will be published in the FACET Newsletter. FACET is issued electronically or can be downloaded from the DACG website. An overview of the DACG correspondents can be found on the DACG website.

WBTR

Since 1st July 2021, associations need to comply with the WBTR-regulation (Wet Bestuur en Toezicht Rechtspersonen). The DACG Board contacted NNV and KNCV and received input and advice regarding potential modifications in the statutes of the DACG. This also holds for the Stichting "International Conferences on Crystal Growth".

Stichting "International Conferences on Crystal Growth"

Two of the Board members of the Stichting "International Conferences on Crystal Growth" (Joop ter Horst and Peter Daudey) were replaced. Currently the Stichting Board consists of the DACG Board members.

¹ The Fall meeting in October 2020 was cancelled and in April 2021 the Spring Meeting was organized online (no symposium fee), so no additional "calendar year" members resulted from these events.



Website

The DACG website (<u>www.dacg.nl</u>, hosted by Radboud University Nijmegen) provides information regarding the structure and activities of the association. All issues of the FACET Newsletter since 2000 are available electronically; links to Dutch research groups in the area of crystallization are available as well as those of foreign DACG 'sister' associations. We welcome any suggestions for improvements; please contact Dr Hugo Meekes (h.meekes@science.ru.nl).

KNCV Piet Bennema Crystal Growth Award 2021

In January 2021 a call for nominations for the KNCV Piet Bennema Crystal Growth Award 2021 was issued and three nominations were received. A jury was installed, consisting of Prof Dominique Maes (Vrije Universiteit Brussel), dr Rob Geertman (Janssen Pharmaceutics) and dr Paul Poodt (TNO), that judged the nominations according to the award requirements. The jury selected dr Jorge Ricardo Cunha as the winner of the 2021 award. Their recommendation was formally approved by the KNCV Board. The other two nominated scientists, dr Sander Brugman and dr Hans Hendrikse, will receive a certificate with an honorable mention. Due to COVID19, the award ceremony has been postponed to April 2022, when we hope to be able to organize a DACG symposium as a "live" event again.

Young-DACG

Marloes Bistervels (PhD student at AMOLF/UvA) approached the DACG Board with an initiative to improve the involvement of specifically the younger researchers (generally PhD students) in the DACG activities, to set up a PhD network and to build an informal bridge between PhD students and group leaders at academia and industry. The platform (to be set up via LinkedIn) also provides a means to exchange communication and discussions on crystal growth related topics as well as an overview of available experimental facilities at universities/industry. A survey and focus session were organized by Marloes which provided feedback on how this platform can be organized efficiently.

Meetings / excursions organized by DACG

On October 9, 2020 the DACG's annual meeting was organized online. The Fall Meeting 2020 was cancelled due to COVID19.

On April 9, 2021 the DACG organized their Spring Meeting online, for the first time. Since this event took place online, the symposium was limited to a timeslot of 2.5 hours in which five speakers gave a presentation on their research.

Activities relevant to DACG community

A shortlist of past activities relevant to the DACG community:

- 9 December 2020: NNV Adviesraadvergadering, online (Hans te Nijenhuis and Antoine van der Heijden attended this meeting on behalf of DACG)
- 9 April 2021: DACG Spring Meeting (online)
- 8 October 2021: DACG Fall Meeting (online)

DACG's 50th anniversary

In 1972 the Kontaktgroep Kristalgroei Nederland (KKN) was established. In 1998, the name was changed in Nederlandse Vereniging voor Kristalgroei, NVKG / Dutch Association for Crystal Growth, DACG. This implies that in 2022 the DACG will celebrate its 50th anniversary. A commission, led by Prof Elias Vlieg, has been founded in 2019 that will start the preparations for organizing an international symposium similar to the BRIDGE symposia held in the past. The previously communicated date for this event (23-25 March 2022) was abandoned due to the fact that several other international crystal growth conferences were postponed to 2022 due to COVID19. The DACG board decided to postpone the 50th anniversary to 2023, in order to prevent too much interference with the other international meetings. Next to NL, UK and Germany, we also intend to invite our Belgian, French and Irish colleagues. Furthermore, the DACG board is looking for other possibilities to celebrate half a century of crystal growth in the Netherlands. For instance, in close cooperation with the editorial board of the Nederlands Tijdschrift voor Natuurkunde (NTvN), a thematic issue on several physics-related aspects of crystal growth will be compiled (2022). DACG members who would like to share their ideas or support the DACG board with the organization of the 50th anniversary of the DACG are most welcome. Please contact the secretary.



Upcoming activities

- 14 October 2021: "Avond van de Chemie" (KNCV event); more information: https://www.kncv.nl/bijeenkomsten/922/avond-van-de-chemie-2021#.YSNdiXzivIU
- December 2021: NNV Adviesraadvergadering (section boards will be invited)
- April 2022: DACG Spring Meeting; University of Utrecht (to be confirmed); date to be decided
- October 2022: DACG Fall Meeting; date/location to be decided



Recent publications

Hans C. Hendrikse, Alejo Aguirre, Arno van der Weijden, Anne S. Meeussen, Fernanda Neira D'Angelo, Willem L.
 Noorduin, Rational design of bioinspired nanocomposites with tunable catalytic activity, Crystals Growth & Design, 2021, 21, 8, 4299–4304.

Affiliations

- AMOLF, Science Park 104, Amsterdam, 1098XG The Netherlands.
- Laboratory of Chemical Reactor Engineering, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands.
- o Leiden Institute of Physics, Leiden University, Niels Bohrweg 2, 2333 CA Leiden, The Netherlands.
- Van't Hoff Institute for Molecular Sciences, University of Amsterdam, 1090 GD Amsterdam, The Netherlands.

Biological assembly processes offer inspiration for ordering building blocks across multiple length scales into advanced functional materials. Such bioinspired strategies are attractive for assembling supported catalysts, where shaping and structuring across length scales are essential for their performance but still remain tremendously difficult to achieve. Here, we present a simple bioinspired route toward supported catalysts with tunable activity and selectivity. We coprecipitate shape-controlled nanocomposites with large specific surface areas of barium carbonate nanocrystals that are uniformly embedded in a silica support. Subsequently, we exchange the barium carbonate to cobalt while preserving the nanoscopic layout and microscopic shape, and demonstrate their catalytic performances in the Fischer–Tropsch synthesis as a case study. Control over the crystal size between 10 and 17 nm offers tunable activity and selectivity for shorter (C_5 – C_{11}) and longer (C_{20+}) hydrocarbons, respectively. Hence, these results open simple, versatile, and scalable routes to tunable and highly reactive bioinspired catalysts.

Hans C. Hendrikse, Stivell Hémon-Charles, Lukas Helmbrecht, Eliane P. van Dam, Eric C. Garnett, Willem L. Noorduin, Shaping tin nanocomposites through transient local conversion reactions, Crystals Growth & Design, 2021, 21, 8, 4500-4505.

Affiliations

- o AMOLF, Science Park 104, Amsterdam, 1098XG The Netherlands.
- o École Polytechnique l'Université de Nantes, 44035 Nantes, France.
- Van't Hoff Institute for Molecular Sciences, University of Amsterdam, 1090 GD Amsterdam, The Netherlands.

Shape-preserving conversion offers a promising strategy to transform self-assembled structures into advanced functional components with customizable composition and shape. Specifically, the assembly of barium carbonate nanocrystals and amorphous silica nanocomposites ($BaCO_3/SiO_2$) offers a plethora of programmable three-dimensional (3D) microscopic geometries, and the nanocrystals can subsequently be converted into functional chemical compositions, while preserving the original 3D geometry. Despite this progress, the scope of these conversion reactions has been limited by the requirement to form carbonate salts. Here, we overcome this limitation using a single-step cation/anion exchange that is driven by the temporal pH change at the converting nanocomposite. We demonstrate the proof of principle by converting $BaCO_3/SiO_2$ nanocomposites into tin-containing nanocomposites, a metal without a stable carbonate. We find that $BaCO_3/SiO_2$ nanocomposites convert in a single step into hydroromarchite nanocomposites ($Sn_3(OH)_2O_2/SiO_2$) with excellent preservation of the 3D geometry and fine features. We explore the versatility and tunability of these $Sn_3(OH)_2O_2/SiO_2$ nanocomposites as a precursor for functional compositions by developing shape-preserving conversion routes to two desirable compositions: tin perovskites ($CH_3NH_3SnX_3$, with $CA_3NH_3SnX_3$



Lukas Helmbrecht, Moritz H. Futscher, Loreta A. Muscarella, Bruno Ehrler, Willem L. Noorduin, <u>Ion Exchange Lithography: Localized Ion Exchange Reactions for Spatial Patterning of Perovskite Semiconductors and Insulators</u>, *Advanced Materials*, 2021, 33, 20, 2005291.

Affiliations

- o AMOLF, Science Park 104, Amsterdam, 1098XG The Netherlands.
- Van't Hoff Institute for Molecular Sciences, University of Amsterdam, 1090 GD Amsterdam, The Netherlands.

Patterning materials with different properties in a single film is a fundamental challenge and essential for the development of next-generation (opto)electronic functional components. This work introduces the concept of ion exchange lithography and demonstrates spatially controlled patterning of electrically insulating films and semiconductors with tunable optoelectronic properties. In ion exchange lithography, a reactive nanoparticle "canvas" is locally converted by printing ion exchange "inks." To demonstrate the proof of principle, a canvas of insulating nanoporous lead carbonate is spatioselectively converted into semiconducting lead halide perovskites by contact printing an ion exchange precursor ink of methylammonium and formamidinium halides. By selecting the composition of the ink, the photoluminescence wavelength of the perovskite semiconductors is tunable over the entire visible spectrum. A broad palette of conversion inks can be applied on the reactive film by printing with customizable stamp designs, spray-painting with stencils, and painting with a brush to inscribe well-defined patterns with tunable optoelectronic properties in the same canvas. Moreover, the optoelectronic properties of the converted canvas are exploited to fabricate a green light-emitting diode (LED), demonstrating the functionality potential of ion exchange lithography.

• Hao Su, Paul H. H. Bomans, Heiner Friedrich, Yifei Xu, Nico Sommerdijk, <u>Crystallization via Oriented Attachment of Nanoclusters with Short-Range Order in Solution</u>, *J. Phys. Chem. C*, **2021**, 125, 1, 1143–1149.

Affiliations

- Laboratory of Materials and Interface Chemistry, Department of Chemical Engineering and Chemistry,
 Eindhoven University of Technology, P.O. Box 513, 5600 MB, Eindhoven, The Netherlands.
- Centre for Multiscale Electron Microscopy, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, P.O. Box 513, 5600 MB, Eindhoven, The Netherlands.
- o Institute for Complex Molecular Systems, Eindhoven University of Technology, P.O. Box 513, 5600 MB, Eindhoven, The Netherlands.
- o Laboratory of Physical Chemistry, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, P.O. Box 513, 5600 MB, Eindhoven, The Netherlands.
- o School of Chemistry, University of Leeds, Woodhouse Lane, LS2 9JT, Leeds, U.K.
- Department of Biochemistry, Radboud Institute of Molecular Life Sciences, Radboud University Medical Center, Geert Grooteplein 6525 GA Nijmegen, The Netherlands.

Many mineral crystallization processes in aqueous solutions involve formation of nanoclusters with short-range order. Their transformation into crystalline products is not well understood. Here we investigate the formation of long-range crystalline order within networks of cobalt-based nanoclusters. High-resolution cryogenic transmission electron microscopy (cryoTEM) together with NMR and FTIR spectroscopies shows the formation of \sim 0.8 nm sized (Co)(NH₃)₅CO₃ complexes at the initial stage. By ligand exchange, those complexes become bridged by CO_3^{2-}/OH^- ligands and form \sim 2 nm sized clusters, which subsequently aggregate into sheetlike networks due to the structural heterogeneity of the clusters. By further ligand change and adjustment in cluster orientations, long-range order is established, which leads to the nucleation of ammonium cobalt kambaldaite nanocrystals. Our observations demonstrate that nanoclusters with short-range order can form crystals via an oriented-attachment pathway, which provides new insights into multistep crystallization processes.



 Mark M. J. van Rijt, Bernette M. Oosterlaken, Heiner Friedrich and Gijsbertus de With, <u>Controlled titration-based</u> <u>ZnO formation</u>, *CrystEngComm*, **2021**, 23, 3340–3348.

Affiliations

 Laboratory of Physical Chemistry, Centre for Multiscale Electron Microscopy, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, P. O. Box 513, Eindhoven, 5600 MB, The Netherlands.

Hexamethylenetetramine (HMTA) is commonly used as a base releasing agent for the synthesis of ZnO under mild aqueous conditions. HMTA hydrolysis leads to gradual formation of a base during the reaction. Use of HMTA, however, does have limitations: HMTA hydrolysis yields both formaldehyde and ammonia, it provides no direct control over the ammonia addition rate or the total amount of ammonia added during the reaction, it results in a limited applicable pH range and it dictates the accessible reaction temperatures. To overcome these restrictions, this work presents a direct base titration strategy for ZnO synthesis in which a continuous base addition rate is maintained. Using this highly flexible strategy, wurtzite ZnO can be synthesized at a pH >5.5 using either KOH or ammonia as a base source at various addition rates and reaction pH values. In situ pH measurements suggest a similar reaction mechanism to HMTA-based synthesis, independent of the varied conditions. The type and concentration of the base used for titration affect the reaction product, with ammonia showing evidence of capping behaviour. Optimizing this strategy, we are able to influence and direct the crystal shape and significantly increase the product yield to 74% compared to the ~13% obtained by the reference HMTA reaction.

• Sevgi Polat, Huseyin Burak Eral, Effect of L-alanyl-glycine dipeptide on calcium oxalate crystallization in artificial urine, Journal of Crystal Growth, 2021, 566–567, 126176.

Affiliations

- Department of Chemical Engineering, Faculty of Engineering, Marmara University, 34722 İstanbul, Turkey.
- Van't Hoff Laboratory for Physical and Colloid Chemistry, Debye Institute for Nanomaterials Science Utrecht University, 3584 CH Utrecht, the Netherlands.
- o Process & Energy Laboratory, Delft University of Technology, 2628 CB Delft, the Netherlands.

Pathological crystallization of calcium oxalate (CaOx), the most common constituent of kidney stones, has attracted much attention due to recent surge in reported natural and synthetic additives effectively inhibiting its nucleation and growth. The aim of this study is to investigate the effect of L-alanyl-glycine (Ala-Gly), a dipeptide commonly found in human urine, on CaOx crystallization and its phase transformation in the presence of an artificial urine media. The nucleated CaOx crystals are characterized by XRD, FTIR, SEM, and dynamic light scattering in terms of changes in their crystalline form, morphology, and size. XRD and FTIR results revealed that Ala-Gly inhibited the formation of the thermodynamically most stable phase of CaOx, calcium oxalate monohydrate (COM) crystals. SEM images revealed that hexagonal plate-shaped COM crystals are transformed into the smaller tetragonal bipyramidal calcium oxalate dihydrate (COD) crystals with increasing additive concentrations. At 125 ppm Ala-Gly concentration more pronounced aggregation of CaOx crystals is observed accompanied with higher negative zeta potential value of -27.1 ± 2.9 mV. Moreover, the phase transformation from COM to COD is also confirmed through thermogravimetric analysis. Consequently, these results suggest that Ala-Gly has a profound effect on preventing the formation of COM crystals and helping to stabilize the COD crystals, a CaOx phase that is reported to have a lower tendency to stick to kidney cells thus decreasing the risk of stone formation. The reported suppression of COM in the presence of Ala-Gly might be significant to clinicians in their attempt to develop a long-term effective treatment for kidney stones.



Frederico Marques Penha, Ashwin Gopalan, Jochem Christoffel Meijlink, Fatma Ibis, Huseyin Burak Eral, <u>Selective Crystallization of D-Mannitol Polymorphs Using Surfactant Self-Assembly</u>, Cryst. Growth Des., **2021**, 21, 7, 3928–3935.

Affiliations

- Department of Chemical Engineering, KTH Royal Institute of Technology, Teknikringen 42, SE100-44 Stockholm, Sweden.
- Process & Energy Department, Delft University of Technology, Leeghwaterstraat 39, 2628 CB
 Delft, The Netherlands.

Selective crystallization of polymorphs is highly sought after in industrial practice. Yet, state-of-the-art techniques either use laboriously engineered solid surfaces or strenuously prepared heteronucleants. We propose an approach where surfactants in solution self-assemble effortlessly into mesoscopic structures dictating the polymorphic outcome of the target solute. Sodium dodecyl sulfate (SDS) surfactant is used as a tailored additive to crystallize different polymorphic forms of a model active pharmaceutical ingredient, d-mannitol. Different mesoscopic phases of SDS template particular polymorphs: packed monolayers, micelles, and crystals favored the β , α , and δ forms of d-mannitol, respectively. A synergistic effect of topological templating and molecular interactions is proposed as the rationale behind the observed selective crystallization of polymorphs. This crystal engineering technique suggests that surfactant self-assemblies can be used as tailored templates for polymorphic control.

 Jason Jung, Roy L. M. Op het Veld, Rik Benoist, Orson A. H. van der Molen, Carlo Manders, Marcel A. Verheijen, Erik P. A. M. Bakkers, <u>Universal Platform for Scalable Semiconductor-Superconductor Nanowire Networks</u>, *Adv. Funct. Mater.* 2021, 2103062 (Early view).

Affiliation

Department of Applied Physics, Eindhoven University of Technology, Eindhoven, MB 5600, The Netherlands.

Semiconductor-superconductor hybrids are commonly used in research on topological quantum computation. Traditionally, top-down approaches involving dry or wet etching are used to define the device geometry. These often aggressive processes risk causing damage to material surfaces, giving rise to scattering sites particularly problematic for quantum applications. Here, a method that maintains the flexibility and scalability of selective area grown nanowire networks while omitting the necessity of etching to create hybrid segments is proposed. Instead, it takes advantage of directional growth methods and uses bottom-up grown indium phosphide (InP) structures as shadowing objects to obtain selective metal deposition. The ability to lithographically define the position and area of these objects and to grow a predefined height ensures precise control of the shadowed region. The approach by growing indium antimonide nanowire networks with welldefined aluminium and lead (Pb) islands is demonstrated. Cross-section cuts of the nanowires reveal a sharp, oxide-free interface between semiconductor and superconductor. By growing InP structures on both sides of in-plane nanowires, a combination of platinum and Pb can independently be shadow deposited, enabling a scalable and reproducible in situ device fabrication. The semiconductor-superconductor nanostructures resulting from this approach are at the forefront of material development for Majorana based experiments.



Elham M. T. Fadaly, Anna Marzegalli, Yizhen Ren, Lin Sun, Alain Dijkstra, Diego de Matteis, Emilio Scalise, Andrey Sarikov, Marta De Luca, Riccardo Rurali, Ilaria Zardo, Jos E. M. Haverkort, Silvana Botti, Leo Miglio, Erik P. A. M. Bakkers, Marcel A.Verheijen, <u>Unveiling Planar Defects in Hexagonal Group IV Materials</u>, *Nano Lett.*, 2021, 21, 8, 3619–3625.

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- Department of Applied Physics, Eindhoven University of Technology, 5600 MB Eindhoven, the Netherlands.
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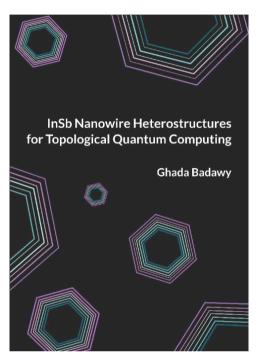
Recently synthesized hexagonal group IV materials are a promising platform to realize efficient light emission that is closely integrated with electronics. A high crystal quality is essential to assess the intrinsic electronic and optical properties of these materials unaffected by structural defects. Here, we identify a previously unknown partial planar defect in materials with a type I_3 basal stacking fault and investigate its structural and electronic properties. Electron microscopy and atomistic modeling are used to reconstruct and visualize this stacking fault and its terminating dislocations in the crystal. From band structure calculations coupled to photoluminescence measurements, we conclude that the I_3 defect does not create states within the hex-Ge and hex-Si band gap. Therefore, the defect is not detrimental to the optoelectronic properties of the hex-SiGe materials family. Finally, highlighting the properties of this defect can be of great interest to the community of hex-III-Ns, where this defect is also present.



PhD theses

 Ghada Badawy, InSb Nanowire Heterostructures for Topological Quantum Computing PhD defense: 8 July 2021, Eindhoven University of Technology, Eindhoven

Promoter: prof. dr. Erik Bakkers Co-promotor: dr. Marcel A. Verheijen



Quantum computing promises to solve certain problems that seemed unsolvable with classical computers. A fundamental challenge, however, is the volatility of information in their building blocks—qubits. Topological quantum computing is considered superior to conventional quantum computing because of the way it stores information. Specifically, a topological quantum computer represents information using quasiparticle excitations known as Majorana fermions. The swapping of these quasiparticles in a material encodes the information such that information is encoded non-locally, protecting it from local sources of noise and decoherence. Among the various platforms that are expected to host Majorana fermions, semiconducting nanowires are considered key contenders. This thesis details the bottom-up growth of indium antimonide (InSb) nanowires and related heterostructures intended as building blocks for the envisioned Majorana-based topological quantum computing circuits.

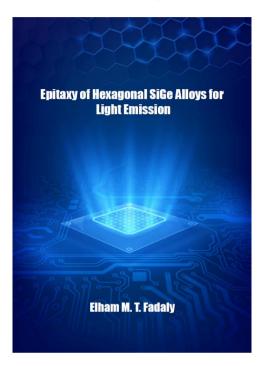
Majorana quasiparticles are predicted to emerge in semiconducting nanowires with strong spin-orbit interaction coupled to a superconductor. The fragility of these quasiparticles demands materials and nanostructures free of any disorder—defects in the nanowire or a rough interface with the superconductor. Another important parameter is the coupling strength between the nanowire and the superconductor which has thus far been largely neglected. The experiments in this thesis improve the InSb nanowires by reducing the impurity levels in them and demonstrate a novel growth method, that allows them to reach lengths that were previously considered unattainable. These nanowires are further refined by including an epitaxial cadmium telluride (CdTe) shell that protects the InSb surface from the surrounding, undesirable electrostatic environment. The growth of an InSb nanostructure, termed a nanoflake, is detailed and is used to selectively deposit the superconductor on the InSb nanowires. To address the coupling strength between the nanowire and the superconductor, we introduce a control knob—the thickness of the same CdTe shell—to modulate the coupling.



Elham M. T. Fadaly, Epitaxy of Hexagonal SiGe Alloys for Light Emission
 PhD defense: 16 April 2021, Eindhoven University of Technology, Eindhoven

Promotor: Prof. E.P.A.M. Bakkers

Co-promotor: Dr. J.E.M. Haverkort, Dr. M.A. Verheijen



Silicon germanium (SiGe) alloys in the hexagonal structure have been theoretically predicted to exhibit a direct band gap nature, *i.e.*, efficient light emission, in the infrared wavelength range 3.5-1.8 μ m. This wavelength range is of technological interest for the optical telecommunications window, which is the basis for fast communication. The fundamental bottleneck is that Si, Ge, and their binary alloys exist naturally in the optically inactive cubic structure. On the other hand, it is extremely challenging to achieve the hexagonal structure in this class of materials.

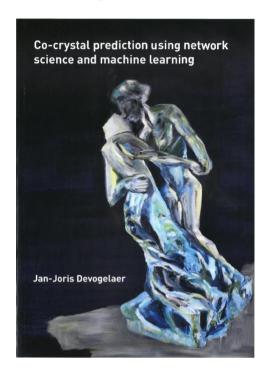
In this thesis, Fadaly has developed high-quality hexagonal Si-based alloys in big volumes, which proved to be capable of emitting light efficiently and having excellent optoelectronic properties. The nanowire geometry offers a unique platform for realizing new crystal structures that are inaccessible except under extreme conditions. She has demonstrated that by changing the arrangement of the atoms of the natural cubic Si structure to the promising hexagonal one. She used hexagonal nanowire templates to transfer the crystal structure to SiGe in a core-shell geometry by utilizing the crystal transfer technique. The high quality crystals reported in this work has enabled the emission wavelength's tunability over a broad range while preserving the superior optical properties by controlling the Si with Ge alloy composition. The Hex-SiGe emission yield is similar to that of direct-bandgap group-III–V semiconductors, the current state-of-the-art laser materials. The finding of this work could potentially lead to the development of the first silicon-based laser or mid-infrared light detectors, both of which would be compatible with the current silicon technology. These lasers could be deployed in several applications such as telecommunications, LiDAR, a radar with laser for self-driving cars, and chemical sensors for medical diagnosis or measuring air and food quality.



 Jan_Joris Devogelaer, Co-crystal prediction using network science and machine learning PhD defense: 17 September 2021, Radboud Universiteit, Nijmegen

Promotor: Prof. dr. Elias Vlieg

Co-promotors: Dr. René de Gelder and Dr. Hugo Meekes



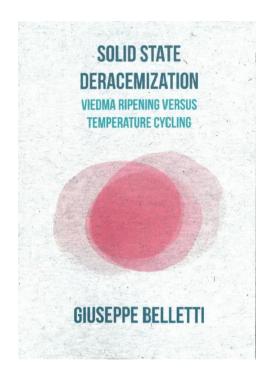
Co-crystallization, the phenomenon where two or more distinct solid compounds form a single crystalline material, has enjoyed a resurgence of interest over the past two decades. The ability to tune physicochemical properties of an underperforming compound, such as the aqueous solubility or hydration stability of a pharmaceutical, together with opportunities regarding controlling polymorphism and chiral separation, have played major roles in its increased popularity. Theoretical tools such as Etter's graph sets and Desiraju's supramolecular synthons have laid the foundation for the current understanding of co-crystal structures in terms of intermolecular interactions. Other decisive factors beyond matching complementary functional groups, however, have stayed relatively unclear. Crystallographic databases such as the Cambridge Structural Database (CSD) contain an abundance of information on co-crystalline systems. Guidelines for the effective design of co-crystals could possibly be unraveled from its content given the right set of tools. The objectives of this thesis are therefore to gain an enhanced understanding of co-crystal formation and to use this to predict new co-crystals using data derived from the CSD. The approaches used to achieve this goal are network science and machine learning.



• Giuseppe Belletti, Solid state deracemization – Viedma ripening versus temperature cycling PhD defense: 27 October 2021, Radboud Universiteit, Nijmegen

Promotor: Prof. dr. Elias Vlieg and Prof. dr. Floris P.J.T. Rutjes

Co-promotor: Dr. Hugo Meekes



Viedma ripening and temperature cycling are known as robust and effective deracemization techniques that use the solid state of chiral compounds. Due to the strict prerequisites, i.e. conglomerate formation and solution racemization, their field of application is a limited range of chiral molecules. Different approaches were used over the past decade to expand the scope of both processes, with the majority focusing on Viedma ripening. In this thesis we study a number of methods to extend the applicability of both processes. In addition, we investigate the consequences of combining Viedma ripening and temperature cycling on the same chiral system. Finally, we introduce a new mechanism that could describe temperature cycling, which is still under debate. The compound used in many studies reported in this thesis is NMPA, which was also the first organic compound used to prove the efficacy of Viedma ripening on a chiral substrate. Much information has been collected over the course of the years on NMPA, therefore making it an ideal model compound.