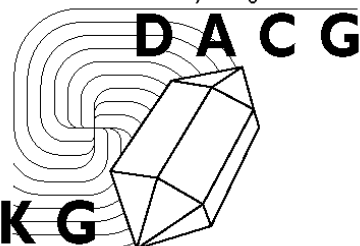


FACET

dutch association for crystal growth



DACG NEWSLETTER

NVKG

nederlandse vereniging voor kristalgroei

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FACET

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Association for Crystal Growth

(DACG), section of the KNCV and

the NNV.

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Cover figure

Salt creeping as a self-amplifying crystallization process.

Image from the group of Dr. Noushine Shahidzadeh, Institute of Physics-WZI, University of Amsterdam. See List of publications for details.

From the editor

New year, new opportunities.

The DACG fall meeting was held in Eindhoven in October. Full coverage is included!

The preparations for our 50-year jubileum have started. Take a look at that!

And again we have included a long list of publications and thesis.

Also, do not forget, the spring symposium is on Friday April 3rd in Utrecht! Sign in by March 23rd, 2020!

As always, it is easy to contribute to the FACET: recently published articles and theses, photos for cover figure, relevant announcements, ... Contributions may be delivered by mail, [e-mail](#), or telephone. Your ideas are welcome, please notify the editor: [Marketta Uusi-Penttilä](#)

Marketta Uusi-Penttilä

Membership

Becoming a member of the DACG is easy: send an e-mail message to [Antoine van der Heijden](#).

The annual membership fee in 2020 is € 15 for professionals, € 10 for 65+ and € 5 for (PhD) students.

Participating in one of the biannual symposia for the first time automatically includes a membership for the ongoing and following year. Members also participate our symposia for a reduced rate.

Upcoming events

- [DACG Spring Meeting](#), 3 Apr 2020, Utrecht.
 - [DACG Fall Meeting](#), 9 Oct 2020, Geleen
-

Report DACG symposium 4 October 2019

On 4 October, 2019, the DACG organized its fall meeting “*Electron microscopy for crystal growth studies*” at ThermoFisher Scientific in Eindhoven. Local organizer and host was Nico Clemens. After the opening of the symposium by Hans te Nijenhuis and Nico Clemens, the first lecture was given by Daniel Phifer giving the audience a brief historic overview of ThermoFisher Scientific company as well as an introduction in scanning and transmission electron microscopy. After this opening lecture, Hans Raaijmakers – also from ThermoFisher Scientific – continued on micro-electron diffraction, being a relatively new application in electron microscopy. Laura Spix from Aspen Oss presented on the important role SEM plays in troubleshooting and process optimization of an active pharmaceutical ingredient (API) that they produce. Due to absence of the originally scheduled speaker Paolo Accordini from Radboud University Nijmegen, René de Gelder (of the same university) kindly offered to present results on the pitfalls, challenges and solutions of the so-called crystalline sponge method. And last-but-not-least, Marcel Verheijen (TU Eindhoven) presented TEM studies on nanoparticles, nanowires and 2-D materials.



Daniel Phifer (ThermoFisher Scientific): *Introduction in electron microscopy*



Hans Raaijmakers (ThermoFisher Scientific): *Micro-Electron Diffraction: a new application in electron microscopy*



Laura Spix (Aspen Oss): *SEM in troubleshooting / process optimization*



René de Gelder (Radboud University Nijmegen): *The crystalline sponge method: pitfalls, challenges and solutions*



Marcel Verheijen (TU Eindhoven): *0-D, 1-D and 2-D crystal growth; TEM studies of nanoparticles, nanowires and 2-D materials*

During the fall symposium, the DACG traditionally holds its annual meeting. This meeting was held directly after lunch.

The symposium concluded with a lab tour during which the participants received a glimpse of the impressive Clean Room facilities and the manufacturing process of transmission electron microscopes at ThermoFisher Scientific in Acht.



The DACG symposium was attended by 35 participants. On behalf of the DACG board, we would like to acknowledge Nico Clemens and his colleagues for their support in the organization of this successful symposium and for hosting the DACG community at ThermoFisher Scientific.

Antoine van der Heijden

Annual membership fee 2020

Just a friendly request for all members to check that you have paid your membership fee for 2020. Being a member you can participate our symposia for a reduced price.

The membership fee in 2020 is € 15 for professionals, € 10 for 65+ and € 5 for (PhD) students. Please mention "DACG membership fee 2020" in your payment.

The bank account of the NVKG is:
Ned. Ver. Van Kristal Groei.
NL60INGB0004305158

*The annual membership runs from 1 January 20XX to 31 December 20XX.
Participating in one of the two annual DACG symposia paying the full participation fee includes the membership for that year (20XX) and the following calendar year (20XX + 1).*

Upcoming DACG 50th anniversary

Dear members of the DACG,

As you might have already heard or read elsewhere, the DACG will celebrate its 50th birthday in 2022. As board, we have started the preparations for this special anniversary, and to make it a success, we need your help.

Over the last 50 years, the DACG has organized or assisted in organizing many events for a national as well as for an international audience. Every year we come together for our Spring and Annual meetings. And in 1995 and 2008 we welcomed the international communities at the ICCG 11 and the ISIC 17 respectively.

Lots of pictures have been taken at these events. **We would like to ask you to have a look in your archives and send us photos that highlight 50 years of crystal growth events in the Netherlands.** Or probably you have pictures of your historical crystal growth or crystallization installations. Also these photos are very welcome.

You can submit your pictures to [Marketta Uusi-Penttilä](mailto:Marketta.Uusi-Penttila@nva.nl). We are looking forward to your contributions.

Hans te Nijenhuis



ISIC in Maastricht



Group photo of meeting in Almelo

DACG Spring Symposium

University of Utrecht, 3 April 2020

- 09:30 – 10:00 **Registration and coffee**
- 10:00 – 10:10 **Welcome and introduction**
Hans te Nijenhuis / Alfons van Blaaderen
- 10:10 – 10:45 **Surprises in the self-assembly of particles in spherical confinement**
Alfons van Blaaderen (UU, Soft Condensed Matter Group)
- 10:45 – 11:10 **Real-space study of homogeneous crystallization of (nearly) hard sphere colloids by arresting the dispersion**
Anna Nikolaenkova (UU, Soft Condensed Matter Group)
- 11:10 – 11:35 **Nature inspired multi-mineral salts for iron fortification**
Simon Lepinay (UvA, Institute of Physics)
- 11:35 – 12:00 **Machine learning for local structure detection in colloidal systems**
Emanuele Boattini (UU, Soft Condensed Matter Group)
- 12:00 – 13:00 **Lunch**
- 13:00 – 14:00 ***title to be announced***
Michael Engel (University Erlangen-Nürnberg, Germany; guest UU)
- 14:00 – 14:25 **Struvite formation in reject water from anaerobic digestion using thermal hydrolysis process**
Javier Pavez Jara (TU Delft, Fac. CiTG, Sanitary Engineering)
- 14:25 – 14:50 **Simultaneous crystallization: towards solvent and solute recovery**
Fred Marques Penha (TU Delft, Fac. 3mE, Process & Energy)
- 14:50 – 15:05 **Coffee break**
- 15:05 – 15:30 **Thermochemical heat storage using salt alcoholates**
Dirk Kok (RU Nijmegen, IMM Solid State Chemistry)
- 15:30 – 16:20 **Lab visit**
- 16:20 – 17:15 **Drinks / nibbles**

Venue: University of Utrecht, Soft Condensed Matter Group, L.S. Ornsteinlab,
Princetonplein 1, 3584 CC Utrecht
Directions: <https://www.uu.nl/en/leonard-s-ornstein-laboratory>

For registration see next page or visit [DACG website](#).

DACG Spring Symposium

University of Utrecht, 3 April 2020

REGISTRATION FORM

For registration, please complete this form and send the scanned form as an attachment to a.e.d.m.vanderheijden@tudelft.nl, ultimately **by 23 March 2020**.

The symposium fee (including coffee, lunch and drinks) is:

25 EURO for (PhD-)students and DACG members
40 EURO for non-members (you will be offered to be enrolled as a DACG member in 2020-2021)

Payment of symposium fee **preferably by bank transfer:**

Nederlandse Vereniging van Kristal Groei

NL 60 INGB 0004305158

Please mention "DACG Spring Symposium 2020" in your payment.

Another possibility is cash payment at the symposium.

Name (first name and surname): _____

E-mail: _____

Affiliation: _____

Postal address: _____

Postal code: _____

City: _____

Member DACG / (PhD-)student / None of the two (*delete what is not applicable*)

Dietary requirements for lunch:

For details regarding DACG privacy policy see our [website](#).

Recent publications

- M.J. Qazi, H. Salim, C.A.W. Doorman, E. Jambon-Puillet, N. Shahidzadeh, [Salt creeping as a self-amplifying crystallization process](#), *Science Advances* **5** (2019), No. 12, eaax1853.
See also some extra articles written about this paper in [NRC](#) and [Physics World](#).

Affiliation

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Salt creeping is a ubiquitous phenomenon in which crystals precipitate far from an evaporating salt solution boundary, which constitutes a major problem in outdoor electronics, civil engineering, artworks, and agriculture. We report a novel experimental approach that allows to quantitatively describe the creeping mechanism and demonstrate its universality with respect to different salts. We show that there exists a critical contact angle below which salt creeping occurs, provided also the nucleation of multiple crystals is favored. The precipitation of new crystals happens ahead of the contact line by the meniscus that progressively advances over the crystals forming also nanometric precursor films. This enlarges the evaporative area, causing an exponential increase in the crystal mass in time. The self-amplifying process then results in a spectacular three-dimensional crystal network at macroscopic distances from the solution reservoir. These findings also allow us to control the creeping by using crystallization modifiers.

- G. Mirabello, A. Keizer, P. H. H. Bomans, A. Kovacs, R. E. Dunin-Borkowski, N. A. J. M. Sommerdijk, H. Friedrich, [Understanding the Formation Mechanism of Magnetic Mesocrystals with \(Cryo-\)Electron Microscopy](#), *Chem. Mater.*, **31** (2019), 7320-7328.

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- Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute, Forschungszentrum Jülich, 52428 Jülich, Germany

Magnetite (Fe₃O₄) nanoaggregates with a flower-like morphology are considered promising materials in the field of magnetically induced hyperthermia in cancer therapy due to their good heating efficiency at low applied alternating magnetic fields. Although the structure and the magnetic state of such flower-like aggregates have been investigated previously, the mechanism that leads to the hierarchical morphology is still poorly understood. Here, we study the formation mechanism of Fe₃O₄ aggregates synthesized through the partial oxidation of ferrous hydroxide in the presence of poly(acrylic acid) by using cryogenic electron microscopy. The aggregates are formed through a multistep process involving first the conversion of ferrous hydroxide precursors in similar to 5 nm primary particles that aggregate into similar to 10 nm primary Fe₃O₄ crystals that finally arrange into the secondary mesocrystal structure. High-resolution electron tomography is used to show that the Fe₃O₄ mesocrystals are composed of similar to 10 nm subunits, often showing a uniform crystallographic orientation resulting in single-crystal-like diffraction patterns. Furthermore, electron holography reveals that mesocrystals have a single magnetic domain despite polymeric interfaces between subunits being present throughout the mesocrystal. Our findings could be used to design materials with specific properties by modulating the morphology and/or magnetic state that is suitable for biomedical application.

- G. Mirabello, A. Ianiro, P.H.H. Bomans, T. Yoda, A. Arakaki, H. Friedrich, G. de With, N.A.J.M. Sommerdijk, [Crystallization by particle attachment is a colloidal assembly process](#), *Nat. Mater.*, (2019)

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- Institute for Complex Molecular Systems, Eindhoven University of Technology, Eindhoven, The Netherlands
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- Division of Biotechnology and Life Science, Institute of Engineering, Tokyo University of Agriculture and Technology, Tokyo, Japan

The nucleation of crystals has long been thought to occur through the stochastic association of ions, atoms or molecules to form critical nuclei, which will later grow out to crystals. Only in the past decade has the awareness grown that crystallization can also proceed through the assembly of different types of building blocks, including amorphous precursors, primary particles, prenucleation species, dense liquid droplets or nanocrystals. However, the forces that control these alternative pathways are still poorly understood. Here, we investigate the crystallization of magnetite (Fe_3O_4) through the formation and aggregation of primary particles and show that both the thermodynamics and the kinetics of the process can be described in terms of colloidal assembly. This model allows predicting the average crystal size at a given initial Fe concentration, thereby opening the way to the design of crystals with predefined sizes and properties.

- W. de Poel, P.T. Tinnemans, A.L.L. Duchateau, M. Honing, F.P.J.T. Rutjes, E. Vlieg, R. de Gelder, [The crystalline sponge method in water](#), *Chem. Eur. J.* **25** (2019), 14999-15003.

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The crystalline sponge method entails the elucidation of the (absolute) structure of molecules from a solution phase using single-crystal X-ray diffraction and eliminates the need for crystals of the target compound. An important limitation for the application of the crystalline sponge method is the instability of the available crystalline sponges that can act as host crystals. The host crystal that is most often used decomposes in protic or nucleophilic solvents, or when guest molecules with Lewis basic substituents are introduced. Here a new class of (water) stable host crystals based on f-block metals is disclosed. It can be shown that these hosts not only increase the scope of the crystalline sponge method to a wider array of solvents and guests, but that they can even be applied to aqueous solutions containing hydrophilic guest molecules, thereby extending the crystalline sponge method to the important field of water-based chemistry.

- J.J. Devogelaer, S.T. Brugman, H. Meekes, P. Tinnemans, E. Vlieg, R. de Gelder, [Cocrystal design by network-based link prediction](#), *CrystEngComm*, **21** (2019) 6875-6885,

Affiliation

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Cocrystallization is an attractive formulation tool for tuning the physicochemical properties of a compound while not altering its molecular structure and has gained interest from both industry and academia. Although the design strategy for cocrystals has marked several milestones over the past few decades, a holistic approach that utilizes as much cocrystal data as possible is still lacking. In this paper, we describe how information contained in the Cambridge Structural Database (CSD) can be used to construct a data-driven cocrystal prediction method, based on a network of coformers and link-prediction algorithms. Experimental validation of the method leads to the discovery of ten new cocrystal structures for its top ten predictions. The prediction method is not restricted to compounds present in the CSD: by combining the information of only a few cocrystals of an unknown coformer (e.g. an API in development) together with the information contained in the database, a set of relevant cocrystal candidates can be generated.

- R. Oketani, F. Marin, P. Tinnemans, M. Hoquante, A. Laurent, C. Brandel, P. Cardinael, H. Meekes, E. Vlieg, Y. Geerts, G. Coquerel, [Deracemization in a complex quaternary system with a second-order asymmetric transformation using phase diagram studies](#), *Chem. Eur. J.*, **25** (2019), 13890-13898.

Affiliations

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- Institute for Molecules and Materials, Radboud University, Heyendaalseweg 135, 6525AJ Nijmegen, The Netherlands

A productive deracemization process based on a quaternary phase diagram study of a naphthamide derivative is reported. New racemic compounds of an atropisomeric naphthamide derivative have been discovered, and a quaternary phase diagram has been constructed that indicated that four solids are stable in a methanol/H₂O solution. Based on the results of a heterogeneous equilibria study showing the stable domain of the conglomerate, a second-order asymmetric transformation was achieved with up to 97 % ee. Furthermore, this methodology showcases the chiral separation of a stable racemic compound forming system and does not suffer from any of the typical limitations of deracemization, although application is still limited to conglomerate-forming systems. We anticipate that this present study will serve as a fundamental model for the design of sophisticated chiral separation processes.

- S.J.T. Brugman, B.L. Werkhoven, E.R. Townsend, P. Accordini, R. van Roij, E. Vlieg, [Monovalent-divalent cation competition at the muscovite mica surface: experiment and theory](#), *J. Coll. Interf. Sci.* **559** (2020) 291-303

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Hypothesis

Ion adsorption on mineral surfaces depends on several factors, such as the mineral surface structure and the valency, size and hydration of the ion. In order to understand competitive adsorption at mineral surfaces, experimental techniques are required that can probe multiple ionic species at the same time. By comparing adsorption of two different cations, it should be possible to derive the factors governing ion adsorption. Divalent cations are expected to bind stronger to the negatively-charged muscovite surface than monovalent cations.

Experiments

Here, the competition between the monovalent Cs^+ and the divalent Ca^{2+} cation for adsorption at the muscovite mica basal plane was investigated using surface X-ray diffraction. Using an extended surface complexation model, we simultaneously fit the measured cation coverages and net surface charges reported in literature.

Findings

In order to reproduce those complementary data sets, both cation adsorption and anion coadsorption were included in the surface complexation model. Moreover, the intrinsic muscovite surface charge and the maximum of available adsorption sites had to be reduced compared to existing literature values. Competition experiments revealed that the affinity of Cs^+ for the muscovite surface is larger than the affinity of Ca^{2+} , showing that hydration forces are more important than electrostatics.

- G. Belletti, C. Tortora, I.D. Mellema, P. Tinnemans, H. Meekes, F.P.J.T. Rutjes, S. Tsogoeva, E. Vlieg, [Photo-racemization based Viedma ripening of a BINOL derivative](#), *Chem. Eur. J.*, **26** (2020), 839-844.

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Viedma ripening is a deracemization process that has been used to deracemize a range of chiral molecules. The method has two major requirements: the compound needs to crystallize as a conglomerate and it needs to be racemizable under the crystallization conditions. Although conglomerate formation can be induced in different ways, the number of racemization methods is still rather limited. To extend the scope of Viedma ripening, in the present research we applied UV-light-induced racemization in a Viedma ripening process, and report the successful deracemization of a BINOL derivative crystallizing as a conglomerate. Irradiation by UV light activates the target compound in combination with an organic base, required to promote the excited-state proton transfer (ESPT), leading thereafter to racemization. This offers a new tool towards the development of Viedma ripening processes, by using a cheap and “green” catalytic source like UV light to racemize suitable chiral compounds.

- Y. Duan, S. Semin, P. Tinnemans, H. Cuppen, J. Xu, T. Rasing, [Robust thermoelastic micro actuator based on an organic molecular crystal](#), *Nature Comm.*, **10** (2019), 4573.

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- School of Materials Science and Engineering, National Institute for Advanced Materials, Nankai University, Tongyan Road 38, 300350, Tianjin, P.R. China

Mechanically responsive molecular crystals that reversibly change shape triggered by external stimuli are invaluable for the design of actuators for soft robotics, artificial muscles and microfluidic devices. However, their strong deformations usually lead to their destruction. We report a fluorenone derivative (4-DBpFO) showing a strong shear deformation upon heating due to a structural phase transition which is reproducible after more than hundred heating/cooling cycles. Molecular dynamic simulations show that the transition occurs through a nucleation-and-growth mechanism, triggered by thermally induced rotations of the phenyl rings, leading to a rearrangement of the molecular configuration. The applicability as actuator is demonstrated by displacing a micron-sized glass bead over a large distance, delivering a kinetic energy of more than 65 pJ, corresponding to a work density of 270 J kg⁻¹. This material can serve as a prototype structure to direct the development of new types of robust molecular actuators.

- P.J. Gilissen, A. Swartjes, B. Spierenburg, J.P.J. Bruekers, P. Tinnemans, P.B. White, F.P.J.T. Rutjes, R.J.M. Nolte, J.A.A.W. Elemans, [Rapid and scalable synthesis of chiral porphyrin cage compounds](#), *Tetrahedron*, **75** (2019) 4640-4647.

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- Radboud University Nijmegen, Institute for Molecules and Materials, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands
- Department of Chemistry, University of Oslo, N-0315 Oslo, Norway

An improved and scalable synthetic route to chiral porphyrin cage compounds, which will be used as catalytic machines for the encoding of information into polymers, has been developed. The porphyrin cage was made chiral by introducing one or two nitro groups on its xylylene sidewalls. This nitration was performed with fuming nitric acid at low temperature and occurred in a highly regioselective fashion. The latter was thought to be the result of the binding of a nitronium cation inside the cavity of the cage compound, directing the reaction to the sidewalls. However, ¹H NMR titrations of the porphyrin cage compound with either nitric acid or the nitronium salt [NO₂][BF₄] revealed that the effect of the host-guest binding of the nitronium ion on the selectivity of the reaction is negligible. Instead, protonation of the porphyrin plays an essential role as it prevents the ring from being oxidized, allowing the nitration to be directed to the sidewalls.

- M. van Eerden, G. Bauhuis, P. Mulder, N. Gruginskie, M. Passoni, L. Andreani, E. Vlieg, J.J. Schermer, [A facile light trapping approach for ultra-thin GaAs solar cells using wet chemical etching](#), *Progr. Photovolt: Res. Appl.* (2019) 1-10.

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- Department of Physics, University of Pavia, Via Bassi 6, Pavia I-27100, Italy

Thinning down the absorber layer of GaAs solar cells can reduce their cost and improve their radiation hardness, which is important for space applications. However, the lighttrapping schemes necessary to achieve high absorptance in these cells can be experimentally challenging or introduce various parasitic losses. In this work, a facile lighttrapping approach based on wet chemical etching is demonstrated. The rear-side contact layer of ultrathin GaAs solar cells is wet-chemically textured in between local Ohmic contact points using an NaOH-based etchant. The resulting contact layer morphology is characterized using atomic force microscopy and scanning electron microscopy. High broadband diffuse reflectance and haze factors are measured on bare and Ag-coated textured contact layers. The textured contact layer is successfully integrated as a diffusive rear mirror in thin-film solar cells comprising a 300-nm GaAs absorber and Ag rear contact. Consistent increases in short-circuit current density (J_{SC}) of approximately 3 mA cm^{-2} (15%) are achieved in the textured cells, while the open-circuit voltages and fill factors do not suffer from the textured rear mirror. The best cell achieves a J_{SC} of 24.8 mA cm^{-2} and a power conversion efficiency of 21.4%. The textured rear mirror enhances outcoupling of luminescence at open circuit, leading to a strong increase in the external luminescent efficiency.

- N. Gruginskie, F. Cappelluti, G.J. Bauhuis, A.P. Cedola, P. Mulder, E.J. Haverkamp, E. Vlieg, [Electron radiation induced degradation of GaAs solar cells with different architectures](#), *Progr. Photovolt: Res. Appl.* (2019) 1-13.

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- Department of Electronics and Telecommunications, Politecnico di Torino, Corso Duca degli Abruzzi 24, Torino, 10129, Italy

The effects of electron irradiation on the performance of GaAs solar cells with a range of architectures is studied. Solar cells with shallow and deep junction designs processed on the native wafer as well as into a thin-film were irradiated by 1-MeV electrons with fluence up to $1 \times 10^{15} \text{ e}^-/\text{cm}^2$. The degradation of the cell performance due to irradiation was studied experimentally and theoretically using model simulations, and a coherent set of minority carriers' lifetime damage constants was derived. The solar cell performance degradation primarily depends on the junction depth and the thickness of the active layers, whereas the material damage shows to be insensitive to the cell architecture and fabrication steps. The modeling study has pointed out that besides the reduction of carriers lifetime, the electron irradiation strongly affects the quality of hetero-interfaces, an effect scarcely addressed in the literature. It is demonstrated that linear increase with the electron fluence of the surface recombination velocity at the front and rear hetero-interfaces of the solar cell accurately describes the degradation of the spectral response and of the dark current characteristic upon irradiation. A shallow junction solar cell processed into a thin-film device has the lowest sensitivity to electron radiation, showing an efficiency at the end of life equivalent to 82% of the beginning-of-life efficiency.

- L. Jacobse, M.J. Rost, M.T.M. Koper, [Atomic-Scale Identification of the Electrochemical Roughening of Platinum](#), *ACS Central Science*, **5** (2019), 1920-1928.

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- DESY NanoLab, Deutsches Elektronensynchrotron DESY, Notkestrasse 85, D-22607 Hamburg, Germany

Electrode degradation under oxidizing conditions is a major drawback for large-scale applications of platinum electrocatalysts. Subjecting Pt(111) to oxidation–reduction cycles is known to lead to the growth of nanoislands. We study this phenomenon using a combination of simultaneous in situ electrochemical scanning tunneling microscopy and cyclic voltammetry. Here, we present a detailed analysis of the formed islands, deriving the (evolution of the) average island growth shape. From the island shapes, we determine the densities of atomic-scale defect sites, e.g., steps and facets, which show an excellent correlation with the different voltammetric hydrogen adsorption peaks. Based on this combination of electrochemical scanning tunneling microscopy (EC-STM) and CV data, we derive a detailed atomistic picture of the nanoisland evolution during potential cycling, delivering new insights into the initial stages of platinum electrode degradation.

- M.J.Rost, L. Jacobse, M.T.M. Koper, [The dualism between adatom- and vacancy-based single crystal growth models](#), *Nature Communications*, **10** (2019): 5233.

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In homoepitaxial crystal growth, four basic growth morphologies (idealized growth modes) have been established that describe the deposition of atoms on single crystal surfaces: step-flow, layer-by-layer, mound formation, and random/self-affine growth. Mound formation leads to nano-scale surface patterning. However, the formation of (nano)-islands, patterns, and roughness occurs also during ion bombardment, electrochemical etching and oxidation/reduction cycling. Here we show, in analogy to many particle/anti-particle formalisms in physics, the existence of the dualism between individual adatom and single vacancy growth modes. We predict that all standard adatom growth modes do exist also in their counter, vacancy version. For the particular case of mound formation, we derive the theoretical equations and show the inverse similarity of the solution. We furthermore treat simultaneous growth by adatoms and vacancies, and derive the analytical solution of the growth shape evolution of the mounds. Finally, we present an experimental verification, in which both adatom and vacancy mound formation are active. The theoretically predicted mound shape nicely fits the experimental observation.

- X. Zhu, G.H. ten Brink, S. de Graaf, B.J. Kooi, G. Palasantzas, [Gas-Phase Synthesis of Tunable-Size Germanium Nanocrystals by Inert Gas Condensation](#), Chem. Mater. 2020, Articles ASAP.

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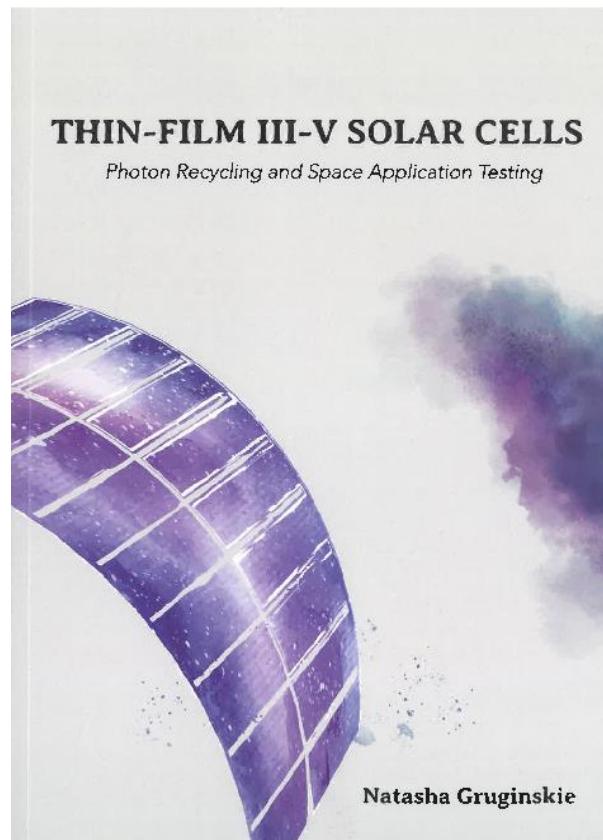
Size-dependent optical properties of germanium (Ge) nanocrystals (NCs) make them a desirable material for optoelectronic applications. So far, the synthesis of ligand-free and tunable-size Ge NCs by inert gas condensation has been scarcely reported. In this work, we introduce a gas-phase approach to synthesize quantum-confined Ge NCs by inert gas condensation, where the size of the Ge NCs can be readily tuned by controlling the thickness of a Cu plate supporting the Ge target. As explained by simulations using the finite element method, the magnetic field configuration above the target can be manipulated by varying the thickness of the Cu backing plate. In-depth analysis based on transmission electron microscopy (TEM) results reveals the morphology and crystalline structure of Ge NCs. X-ray photoelectron spectroscopy has proven the formation of a substoichiometric Ge oxide shell for the as-deposited Ge NCs. In addition, Raman spectroscopy indicated peak shifts according to the phonon confinement model that yielded nanoparticle sizes in a good agreement with the TEM results. Furthermore, the quantum confinement effect for Ge NCs was demonstrated by analysis of the absorption (UV–vis–NIR) spectrum, which indicated that the band gap of the Ge NCs was increased from ~0.8 to 1.1 eV with decreasing size of Ge NCs. Comparison with theory shows that the quantum confinement effect on the band gap energy for different-sized Ge NCs follows the tight-binding model rather well.

PhD theses

- Natasha Gruginskie, Thin-Film III-V Solar Cells -photon recycling and space application testing
PhD defense: 27 January 2020, Radboud Universiteit, Nijmegen

Promotor: Prof.dr. E. Vlieg

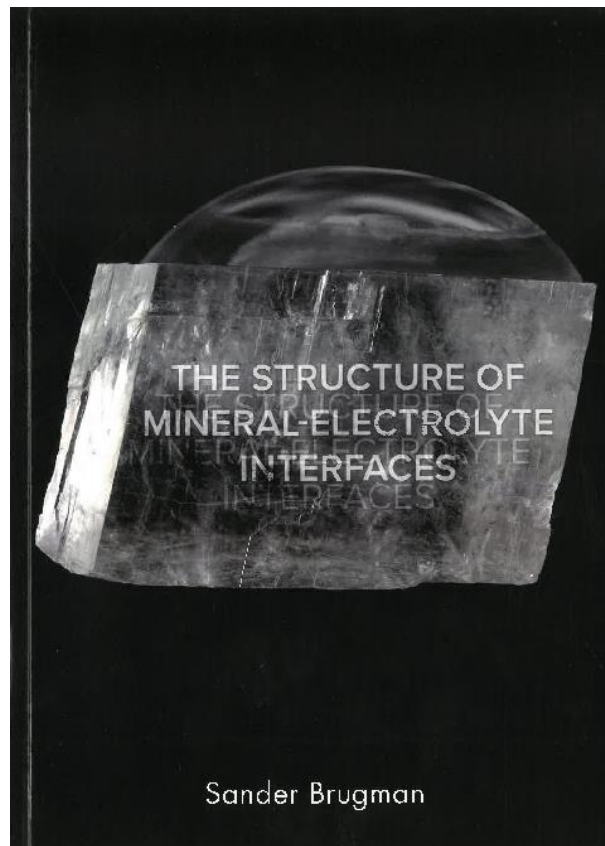
Co-promotor: Dr. Ir. J.J. Schermer



Thin-film GaAs solar cells have several application advantages over cells on their native GaAs or Ge substrate, such as a high power to weight ratio, flexibility, prospects for cost reduction by wafer reuse and possibilities for transferred device applications. These advantages allow the solar cell systems to be optimized to the specific application requirements. Furthermore, it has been shown that the thin-film cells present a superior performance, which is attributed to an increased photon recycling provided by the reflectance of photons at the rear mirror. Because GaAs solar cells quality increased to a point where their performance is limited by radiative recombination, the high internal emissions in these cells make the optical design of the devices to be extremely important. In the thesis, the design and fabrication of thin-film GaAs solar cells is studied, focusing on photon recycling mechanisms and their applicability in space missions.

- Sander Brugman, The structure of mineral-electrolyte interfaces
PhD defense: 18 February 2020, Radboud Universiteit, Nijmegen

Promotor: Prof.dr. E. Vlieg



Surfaces play a big role in many chemical phenomena, such as corrosion, lubrication, adsorption of organic molecules, crystal growth and catalysis. In order to control these processes, a better understanding of the surface structure is required. The surface structure often differs from the structure in the bulk crystal, therefore several techniques have been developed to investigate the surface structure. Surface X-ray diffraction is an excellent technique for determining the structure of interfaces. The large penetration depth of the X-ray beam makes in-situ measurements of solid-liquid interfaces possible. In the thesis several phenomena taking place at the mineral-liquid interface are investigated, mainly using surface X-ray diffraction, but complimented by other methods if possible. Mineral surfaces are important for the study of the origin of life, the adsorption of radioactive particle and for oil recovery, and are therefore relevant subjects of study. In the thesis ion adsorption competition, structuring of hydration water, adsorption of organic molecules and epitaxial crystallization are studied. To do so, some of the largest surface X-ray diffraction data sets were acquired.