Project Description – Project Proposals

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Understandig the wetting behavior of shape memory polymers: Insights from phase-field simulations

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Project Description

1 State of the art and preliminary work

Droplet wetting is an omnipresent phenomenon in nature and engineering applications. For instance, the lotus effect exhibited on leaves is well known to all. In industry, there are a wide range of applications of droplet wetting, such as ink-jet printing, spray cooling, coating and microfluidics [1-4]. For ideal, rigid, mechanically and chemically homogeneous surfaces, the wetting characteristics can be well described by Young's law [5]. However, most of the real surfaces present in nature and industry are chemically and mechanically heterogeneous. Understandings of droplet wetting on real surfaces are difficult because the surface inhomogeneities are generally randomly distributed. These surface inhomogeneities give rise to energy barriers for droplet spreading, most probably leading to multiple local free energy minima [6], which are extremely challenging to be predicted through theoretical analyses. As a global parameter, the equilibrium contact angle on chemically heterogeneous and rough surfaces has been theoretically studied by Cassie [7] and Wenzel [8], respectively. Their models have been widely confirmed both in experiments and simulations.

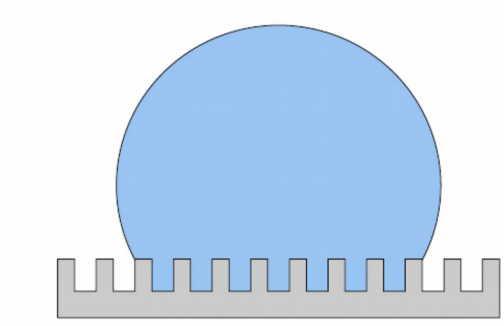

Fig 1: Wenzel state

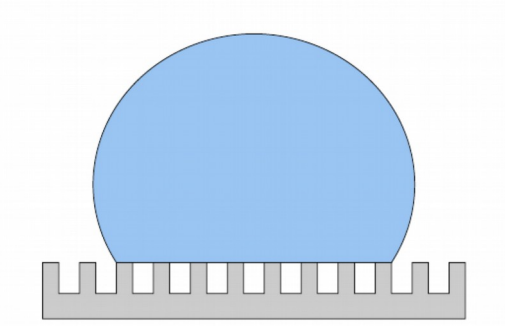

Fig 2: Cassie-Baxter state

With prominent simplifications, wetting on deliberately designed chemically heterogeneous surfaces, such as stripe, chessboard and pizzalike patterned surfaces, has been broadly studied over past years [6,9-11]. In particular, wetting on chemically striped patterned surfaces has attracted considerable interest over the past two decades. For instance, the morphological wetting transitions and instabilities of droplets wetting on chemically striped patterned surfaces have been discussed by a number of authors [12-17].
The anisotropic droplet shapes on chemically striped patterned surfaces have been experimentally and numerically investigated by Bliznyuk et al. [18] and Jansen et al. [19-22], respectively. Furthermore, the droplet spreading dynamics on chemically patterned surfaces are explored by Kusumaatmaja et al. [23] In addition, they discuss the contact angle hysteresis on chemically patterned and superhydrophobic surfaces [6].

They also investigate the anisotropic morphologies of droplets spreading on corrugated surfaces [24]. Most recently, Semprebon et al. [25] focus on the shape evolution of droplets on surfaces with linear microgrooves, showing that the shape evolution of droplets slowly growing on this kind of surface has two distinct morphological regimes. Despite of numerous researches, the current understandings of the underlying mechanisms of droplet wetting and morphological evolution on chemically or mechanically heterogeneous surfaces are still limited. The simulations enable an analysis of surface energies of droplets and can predict the equilibrium shapes of droplets under different conditions.
Various methods for simulating interfacial problems in two-phase flows have been developed over the past decades (see e.g. the review by Wörner [26] and by Sui et al. [27]). Among these methods, the molecular dynamic (MD) and the Monte Carlo (MC) methods are in the atomistic level, the lattice Boltzmann (LB) method is in mesoscale and the phase-field method (PFM) combined with the Navier-Stokes [Se-4] equations belongs to the continuum methods.
Both MD and MC are computationally expensive and thus are restricted to nano- or micro-scale. The scale-bridging nature of LB method is an advantage, but the hydrodynamic boundary conditions are difficult to satisfy on a grid point exactly [26]. The PFM, which is a diffuse interface method, has become very popular to handle the interfacial problem, such as droplet breakup [28], moving contact lines [29] and wetting phenomena [Se-1]. Given that the main focus of our project not only restricted on the equilibrium shapes and will also study the droplet spreading dynamics, the Allen-Cahn-type phase-field model with preserved volume fractions [Se-2] is of great advantage. Compared with the Cahn-Hilliard model [30], the Allen-Cahn model has lower computational load and needs fewer simulation time. Furthermore, a specific wall free energy f_w is embedded into the total free energy in our model, ensuring the right contact angles at triple points. Our model has been experimentally validated [Se-1,Se-3]. Additionally there where applied a study to validate the angle of triple junctions under different modeling configurations [Se-5].

*1.1 **Project-related publications***

1.1.1 **Articles published by outlets with scientific quality assurance, book publications, and works accepted for publication but not yet published.**

[Se-1] Ben Said, M.; Selzer, M.; Nestler, B.; Braun, D.; Greiner, C.; Garcke, H. (2014). A phase-field approach for wetting phenomena of multiphase droplets on solid surfaces. *Langmuir*, *30*(14), 4033-4039.
[Se-2] Nestler, B.; Wendler, F.; Selzer, M.; Stinner, B.; Garcke, H. (2008). Phase-field model for multiphase systems with preserved volume fractions. *Physical Review E*, *78*(1), 011604.
[Se-3] Schweigler, K. M.; Said, M. B.; Seifritz, S.; Selzer, M.; Nestler, B. (2017). Experimental and numerical investigation of drop evaporation depending on the shape of the liquid/gas interface. *International Journal of Heat and Mass Transfer*, *105*, 655-663.
[Se-4] Wang, F.; Choudhury, A.; Selzer, M.; Mukherjee, R.; Nestler, B. (2012). Effect of solutal Marangoni convection on motion, coarsening, and coalescence of droplets in a monotectic system. *Physical Review E*, *86*(6), 066318.
[Se-5] Hötzer, J.; Tschukin, O.; Said, M. B.; Berghoff, M.; Jainta, M.; Barthelemy, G.; Smorchkov N.; Schneider D.; Selzer M.; Nestler, B. (2016). Calibration of a multi-phase field model with quantitative angle measurement. *Journal of materials science*, *51*(4), 1788-1797.

1.1.2 **Other publications**

[Se-6] Sandfeld, S.; Dahmen, T.; Fischer, F. O.R.; Eberl, C.; Klein, S.; Selzer, M.; Nestler, B.; Möller, J.; Mücklich, F.; Engstler, M.; Diebels, S.; Tschuncky, R.; Prakash, A.; Steinberger, D.; Kübel, C.; Herrmann, H.-G.; Schubotz, R.; Digitale Transformation in der Materialwissenschaft und Werkstofftechnik Strategiepapier (https://www.dgm.de/medien/print-medien/strategiepapier-digitale-transformation/)

1.1.1 **Patents**

1.1.2.1 **Pending**

No patents are pending.

1.1.2.2 **Issued**

No patents are issued.

2 Objectives and work programme

2.1 Anticipated total duration of the project

The proposed duration of the project is 36 month.

2.2 Objectives

The coupling of a liquid with a dynamic, switchable substrate is a fascinating research topic as the fundamental physics behind such interactions are far from being fully understood. This is true for simple liquids like water and as well for mixtures of immiscible liquids.
In this project, we will study how a liquid droplet interacts with a switchable fibrillar surface by using phase-field models [Se-1]. These substrates are fabricated following Reedy et al. [33], employing a photolithographic texturing route and a shape memory polymer. This allows switching the fibers (diameter 10 µm and with an aspect ratio of four) from upright to a tilted geometry by 45° through a variation of the substrate temperature. A second mode of actuation is implemented by embedding ferromagnetic nanoparticles into Polydimethylsiloxane (PDMS) fibers [34, 35]. These fibers (same dimensions as with the shape memory polymer) will be actuated by an external magnetic field. This approach allows switching the pillars by about 70° back and forth; if needed with frequencies of several Hertz. The benefit of the magnetic actuation is that the entire knowledge on how to modify and control PDMS can be applied. This includes changes in stiffness by at least an order of magnitude and control over the surface chemistry, e.g. by silanization.

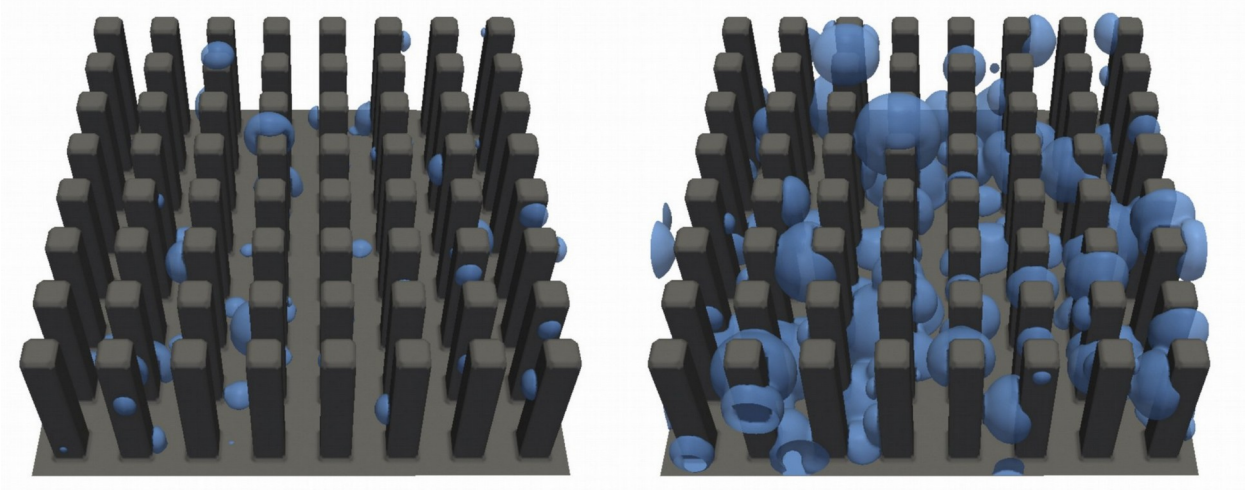

Fig 3: Condensation on chemical homogenious pillars

The simulation results like the previous studies in Fig. 3 and Fig. 4 will open the door for a much deeper understanding of the physics underlying wetting and substrate dynamics. Therefor we aim to calibrate the simulation methods by experimental results

and use that model to predict the behavior of different setups of shape memory polymers. This enables to explore the parameter space by quantitative simulation methods without expensive experiments. This knowledge is of vital importance in modern microfluidic devices and for additive manufacturing.
Even if the main focus of the project is to model the change of the substrate morphology there will be also a focus on chemical change of the surface within the SPP 2171. This will be done in cooperation with experimentally working groups like the mentioned groups in section 5.4.1 but also other groups with a strong interest in modeling of experimental setups.

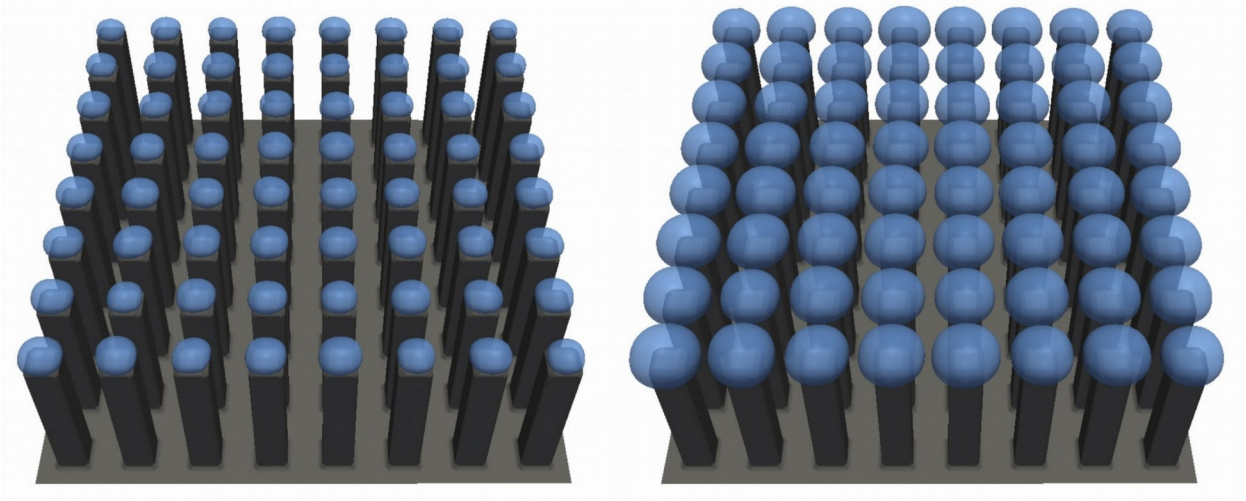

Fig 4: Pillars with chemical heterogenious surface

*2.3 **Work programme incl. proposed research methods***

The phase-field method (PFM) based on the Allen-Cahn model will be used to simulate the droplet behavior on chemically and mechanically treated surfaces. We consider a two-phase system with liquid and gas phases, denoted by l and g, respectively. We introduce a vector-valued continuous order parameter $\varphi(x, t) = (\varphi_l(x, t), \varphi_g(x, t))$ to describe the state of the phases. By postulating the constraint $\varphi_l(x, t)+\varphi_g(x, t) = 1$, the phase-field order parameters $\varphi_l(x, t)$ and $\varphi_g(x, t)$ can be interpreted as the local volume fractions of the liquid and the gas phases, respectively. By defining $\varphi_l := \varphi$, we have $\varphi_g = 1-\varphi$. Then, $\varphi=1$ and $\varphi=0$ represent the pure liquid and the pure gas phases, respectively. The order parameter φ varies continuously from 0 to 1 across the liquid-gas interface. We model the equilibrium properties of the droplet by an energy density functional [Se-1,Se-3]:

$$F(\varphi)=\int_{\Omega} w(\varphi)+\varepsilon a(\varphi,\nabla\varphi)+f_{driv}(\varphi)+g(\varphi)\,d\Omega+\int_{S} f_w(\varphi)\,dS \qquad (1)$$

where Ω is the spatial domain and S indicates the solid-fluid boundary. ε is a modeling parameter related to the thickness of the diffuse interface. The first term in Equation (1) is an obstacle potential, which is formulated as

$$w(\varphi)=\begin{cases}\dfrac{16}{\pi}\gamma_{lg}\varphi(1-\varphi) \; if \; \varphi\in[0,1]\\ \infty \; else\end{cases} \qquad (2)$$

where γ_{lg} is the liquid-gas surface tension. The second term in Equation (1) denotes the gradient energy density which is expressed as

$$a(\varphi, \nabla\varphi) = \gamma_{lg} |\nabla\varphi|^2 \qquad (3)$$

The third term $f_{driv}(\varphi)$ in Equation (1) depicts the bulk free energy density contribution, which is responsible for the phase transition, i.e. evaporation and condensation. During the evaporation and condensation processes, the droplet volume is decreased or increased slowly enough so that the dynamic effects are reduced and thus, at each time, the droplet can be considered as in a state of equilibrium. Lukyanov et al. [36] have proved that the droplet interfaces are expected to be at equilibrium in slow hydrodynamic motion. The driving force for phase transition is described in terms of water concentration gradient

$$f_{driv}(\varphi) = p(c_s - c_p)h(\varphi) \quad (4)$$

here p, cs, and cp are the ambient pressure, saturation and current concentration of water in the gas phase, respectively. h(φ) is an interpolation function and reads

$$h(\varphi) = \varphi^3(6\varphi^2 - 15\varphi + 10) \quad (5)$$

We set f_{driv} (φ) as 0, if the droplet volume is constant, i.e. without evaporation and condensation. For the situation with phase transition, we use different values of the current water concentration c_p to get a positive or negative value of $f_{driv}(\varphi)$ corresponding to the evaporation and condensation, respectively.
The fourth term in Equation (1) indicates a bulk energy density contribution discussed in detail in [Se-2,32]

$$g(\varphi)=\sum_{\alpha=1}^{2} \chi_\alpha h(\varphi_\alpha) \quad (6)$$

with weight function χ_α. g(φ) ensures that the volume change is only due to the contribution of $f_{driv}(\varphi)$. The last term in Equation (1) describes the interaction between the liquid/gas and the solid substrate. The solid-fluid interfacial energy density is formulated as

$$f_w(\varphi) = \gamma_{ls} + (\gamma_{gs} - \gamma_{ls})h(\varphi), \quad (7)$$

where γ_{ls} and γ_{gs} represent the liquid-solid and gas-solid surface tensions, respectively. By minimizing the free energy functional, we obtain the equilibrium state. The evolution of the order parameter φ is derived by the functional derivative

$$\tau\varepsilon \frac{\partial \varphi}{\partial t}=-\frac{\delta F(\varphi)}{\delta \varphi}, \quad (8)$$

where τ is a temporal relaxation parameter for the gas-liquid interface. Using δ/δφ = ∂/∂φ − ∇·(∂/ ∂∇φ), we obtain

$$\tau\varepsilon \frac{\partial \varphi}{\partial t}=2\varepsilon\gamma_{lg}\Delta\varphi-\frac{16}{\varepsilon\pi^2}\gamma_{lg}(1-2\varphi)-p(c_s-c_p)\frac{\partial h(\varphi)}{\partial \varphi}-\frac{\partial g(\varphi)}{\partial \varphi}\ \text{in}\ \Omega \quad (9)$$

with the boundary condition

$$2\varepsilon\gamma_{lg}\frac{\partial \varphi}{\partial n}=(\gamma_{gs}-\gamma_{ls})\frac{\partial h(\varphi)}{\partial \varphi}\ \text{on}\ S \quad (10)$$

where n denotes the normal vector of the solid-fluid boundary S. The boundary condition Equation (10) leads to the Young's law cos θ = $(\gamma_{gs} - \gamma_{ls})/\gamma_{lg}$, which is discussed in detail by Xu et al. [31]. Here, θ is the equilibrium contact angle. To investigate the equilibrium shapes of droplets and the droplets are at equilibrium during the whole condensation and evaporation processes, this boundary condition is chosen for our simulations. For the general case where the droplets at each time step are not in an equilibrium state, the corresponding boundary

condition has been formulated by Jacqmin [32]. Equations (9) and (10) are discretized by the finite difference method with an explicit Euler time marching scheme. The simulations will be performed in 3D geometries by using an equidistant mesh with a spacing of $\Delta x = \Delta y = \Delta z$ as well as adaptive grid resolutions.

WP-1: **Extension of the phase-field model for switchable substrates**
The existing phase-field model from eq. (1) needs to be extended to be able to describe the change of the mechanical structured surface over time. As the influences on the surface can have different sources like change of pH level or some mechanical or chemical influences this will be modeled as a general extension of the used boundary condition to be a function of different properties, i.e. time.

WP-2: **Validation and simulation study of the model for switchable substrates**
The extended boundary condition from WP-1 will be used to model and study the influence of the changed geometry of the surface on the nucleation and transport behavior of liquid droplets. The variation of diameter and the degree of bending of the pillars will be investigated to predict their influence on the droplet.

WP-3: **Optimization of the model for large/real applications**
The ration between the droplet and the structure of the surface has in almost any real application several orders of magnitute. To get insights in this configurations we will develop methods to handle this numerically in an efficient way. This will be done by evaluating homogenization methods as well as adaptive numerical schemes to reduce the calculation time of the simulation setups in a way that large simulation series are possible in a realistic time schedule.

WP-4: **Extent the applications to research within the SPP 2171**
Within this project we will not only focus on the discussed treatment of the surface by magnetic fields. As an important goal we will study experimental setups of other groups (like the groups listed in section 4.4.1) within the SPP 2171 to understand the relevant mechanism of their setups and to extent the existing phase-field model and the boundary condition to capture the physics behind this experiments on the mesoscopic scale.

WP-5: **Converting and preparation of experimental data**
Utilize data from experimentalists for the comparison with the simulation results. This should be done in cooperation with the experimentalists within the SPP 2171. Data from publications and experimental data sets needs to be converted and prepared by filters and other algorithms to get statistics for to compare the experimental and simulation results, i.e. principle component analysis (PCA).

		1-1	1-2	1-3	1-4	2-1	2-2	2-3	2-4	3-1	3-2	3-3	3-4
WP-1	*Extension of the phase-field model*	■	■	■									
WP-2	*Validation and simulation study*			■	■	■	■						
WP-3	*Optimization of the model*						■	■	■	■			
WP-4	*Extent the research within the SPP*								■	■	■	■	■
WP-5	*Converting and preparation of experimental data*	■	■	■	■	■	■	■	■	■	■	■	■

Fig 5: Gantt-chart für the project for each quarter during the project time.

2.4 Data handling

In the recent years we have developed an infrastructure at the institute IAM-CMS to handle large amount of data from simulation results and to compare this with experimental data sets. This large amount of data has the need to have a fast network access (~10GBit/s) to the data sets on RAID-Systems (effective storage size of >50TByte). We have established a workspace concept which makes it possible to manage large amount of data sets across different networks, different storage systems and archive them after all needed processing and analyzing steps on the large scale data facility (LSDF) at the compute center of the KIT for at least 10 years. Further more we are working on the accessibility to data sets by establishing data repositories to make the data accessible to researchers outside the institute. In general the project will follow the statements given in the strategy paper of the Deutsche Gesellschaft für Materialkunde e.V. (DGM) [Se-6].

2.5 Other information

Please use this section for any additional information you feel is relevant which has not been provided elsewhere.

None

2.6 Descriptions of proposed investigations involving experiments on humans, human materials or animals as well as dual use research of concern

This is not relevant in this project.

2.7 Information on scientific and financial involvement of international cooperation partners

There is no financial involvement of international cooperation.

3 Bibliography

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4 Requested modules/funds

4.1 Basic Module

4.1.1 Funding for Staff

The proposed founding is for a PhD student 75 % position (48.375 € per year) for three years. The person in charge will be responsible for the WP-1-4 and will superwise the WP-5. The WP-5 will be handled by a student assistant (6.000 € per year) over the full project time of three years.

Total costs of the project for the staff will be 3 years * 48.375 € + 3 years * 6.000 € = 163.125 €

4.1.2 Direct Project Costs

none

4.1.2.1 Equipment up to Euro 10,000, Software and Consumables

No equipment is needed.

4.1.2.2 Travel Expenses

For traveling to collaborating groups within the SPP 2171 for scientific exchange and further discussion we estimate 2.500 € per year. This includes 1-2 meetings within the SPP, with 1-2 meetings with cooperating partners and one national/international conference including conference fee per year.

4.1.2.3 Visiting Researchers (excluding Mercator Fellows)

No cost for visiting researchers

4.1.2.4 Expenses for Laboratory Animals

No expense for laboratory animials

4.1.2.5 Other Costs

No other costs.

4.1.2.6 Project-related publication expenses

It is planned to publish in OpenAcces journals. The assumed cost per publication is 2500 €. As it is expected to have at least one publication per year in an OpenAccess journals we request 7.500 € for the whole project.

4.1.3 Instrumentation

4.1.3.1 Equipment exceeding Euro 10,000

No instruments needed.

4.1.3.2 Major Instrumentation exceeding Euro 50,000

Not needed.

4.2 Module Temporary Position for Principle Investigator

Not needed.

4.3 Module Replacement Funding

Not needed.

4.4 Module Temporary Clinician Substitute

Not needed.

4.5 Module Mercator Fellows

Not needed.

4.6 Module Workshop Funding

Not needed.

4.7 Module Public Relations Funding

Not needed.

5 Project requirements

5.1 Employment status information

Michael Selzer, fix-term, Helmholtz founded

5.2 First-time proposal data

Not applicable.

5.3 Composition of the project group

Michael Selzer, Dr.-Ing., fixed position, Helmholtz founded
Britta Nestler, Prof. Dr., fixed position, founded by state
Fei Wang, Dr.-Ing., limited position, Helmholtz founded
Andreas Reiter, Phd-Candidate, fixed position, third-party founded
Johannes Hötzer, Dr.-Ing., fixed position, third-party founded

5.4 Cooperation with other researchers

5.4.1 Researchers with whom you have agreed to cooperate on this project

Within the SPP it is planned to cooperate with Frank A. Müller, Friedrich-Schiller-Universität Jena to use their experimental data sets of strain-dependent wetting to perform phase-field simulations of transport processes on the micro- and mesoscale.
Additional cooperation is planned with the group of Popp and Hager, Friedrich-Schiller-Universität Jena, who will provide data obtained from the contact angle measurements (*e.g.,* surface tension). Additionally, the information about the underlying kinetics revealed by CARS spectroscopy and contact angle investigations will also be utilized to perform theoretical simulations on wetting phenomena. Consequently, a correlation of theoretical and experimental data will be accessible gaining a detailed understanding of the wetting behavior of the polymer systems.

5.4.2 Researchers with whom you have collaborated scientifically within the past three years

Lorenz Ratke, DLR
Jürgen Brillo, DLR
Christoph Hilgers, KIT
Thomas Kohl, KIT
Harald Garcke, Universität Regensburg

5.5 Scientific equipment

The hosting institute IAM-CMS at KIT contains a large computational working schedule so that substantial amounts of computer resources (computing time, random access memory (RAM) and main hard disk storage) is needed. The following computer equipments are available for the project: high-performance Linux-Cluster with 90 nodes and 720 Opteron Cores and 1,4 TByte RAM, Infiniband network, 1GBit Ethernet. From each desk, the users in the research group have access to 28 TByte data storage installed with a parallel file system Lustre - a research computer poolroom with 40 dual core opteron processor workstations and a RAID storage system of 4 TByte. Furthermore, the institute has access to high performance computers ForHLR2 at the Scientific Computing Center at KIT which can also be used for simulations.

5.6 Project-relevant cooperation with commercial enterprises

If applicable, please note the EU guidelines on state aid or contact your research institution in this regard.

There is no cooperation with commercial enterprises planed within this project.

5.7 Project-relevant participation in commercial enterprises

Information on connections between the project and the production branch of the enterprise

There is no project relevant participation in commercial enterprises.

6 Additional information

If applicable, please list proposals requesting major instrumentation and/or those previously submitted to a third party here.

A request for funding of this project has not been submitted to any other institution. If we do submit such a request, we will immediately inform the DFG. Rules of good scientific practice: In submitting this proposal for a research grant to the DFG, we agree to adhere to the DFG's rules of good scientific practice. In preparing this proposal, we have adhered to the guidelines for publication lists and bibliographies.