Report on the ICMS workshop "Dynamical Problems in Mathematical Materials Science"

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Significant deviations from the original proposal. None.

Short description of the meeting. Over the past 20 years, mathematical materials science has become a vibrant discipline, with a very significant impact both on mathematics and materials science:

- On the one hand, materials science provides a very rich source of problems in various areas of mathematics. For example, the link between the microscopic structure and macroscopic properties can be explored by certain mathematical techniques, namely homogenisation and relaxation. Over the past few decades this has led to substantial progress in both numerical and mathematical analysis. Mathematical progress, especially in the context of the calculus of variations, has produced a good understanding of several *static* problems.
- On the other hand, the field of materials science has been and continues to be revolutionised by the availability of experimental and theoretical advances in multiscale methods based on advanced mathematics. The newly gained ability to design materials with intricate features on an almost atomistic level calls for a theoretical foundation.

The challenge is to understand the *dynamics* of multiscale problems in materials science, and how dynamics on one scale affect those on the other. Activities in this field are now just emerging and were the theme of this conference.

Comprehensive report of the workshop

Structure of the workshop. The workshop was organised in the Oberwolfach style: every participant had to deliver a talk, while the organisers were not allowed to present a talk.

The talks can be attributed to the following three categories, which were about equally strongly represented: (i) microscopic models, (ii) macroscopic models, and (iii) micro-to-macro transition. Though the applications in materials science were deliberately chosen to be mainly confined to phase transitions and plasticity, the mathematical methodology was quite rich as a result of the different scales involved. This diversity made the workshop a challenging one, as noted by several participants.

Scientific highlights of the workshop. A goal of the workshop was to initiate a fruitful exchange between discrete and continuum viewpoints, and similarly between Mechanics, Engineering, Physics, and Mathematics. We feel that these goals were accomplished. This is reflected in the evaluation of the workshop: the "interdisciplinary nature", the "confluence of ideas in mathematics and mechanics", the "interaction between mathematical and material-science viewpoints" and the value of experimental talks for applied mathematicians were mentioned as highlights of the workshop. Other participants regarded the "wide range of models" and in particular the discussion of discrete models as highlights. One of the subjects where the importance of (i) the combination of discrete and continuum models

and (ii) cooperation of engineers and mathematicians was seen to be crucial is motion of dislocations and grain boundaries and plasticity (talks by Carpio, Mielke, and Gottstein).

The lectures were generally seen to be of uniformly high quality; the keynote lectures were praised for providing an "excellent overview of advanced and modern approaches of mathematical materials science".

Several talks (Friesecke, Pego, Carpio, Le Bris, Dreyer) were singled out by some participants as particular highlights. From the organisers' point of view, a highlight was the talk by Gero Friesecke, in which the stability of fcc crystals under a large class of perturbations was proved. This question has, for three space dimensions, been open for decades, if not a century. The stability result was only obtained about a month before the workshop took place. Several other talks presented similarly recent results as well — among them the existence of travelling waves for certain lattice systems (presented by Schwetlick), homogenisation of Hamiltonian systems with wiggly energies (Smyshlyaev and James), the Boltzmann-Grad limit in the linear regime (Theil and Matthies).

Besides the density of interesting talks, the discussions during and after the talks and the possibility to make connections to researchers from all over the world were particularly estimated by the participants. The scientific standing of the participants was generally seen to be very high.

Academic value of the workshop. There seems to be a rather uniform feeling among the participants that the workshop was of very high or excellent academic value. This feeling is shared by the organisers. We were pleased to see intense interactions developing between the participants. In many talks, there were references to previous talks and discussions, such as "I learnt yesterday that there is another way of doing this". The high value results from the mix of participants, who all have a very high expertise, and work in related interdisciplinary fields. The topic of the workshop was seen as "timely, practically relevant and scientifically challenging". We share the feeling of a participant that the contributions represent the "state of the art in mathematical materials science".

Future directions. For this workshop, it was probably reasonable to confine ourselves to only a few selected topics, namely phase transitions and selected problems in dislocation dynamics. Otherwise, the physical capacities of 14 India Street would have been exceeded. We were able to discuss many topics seen as key future directions by the participants: modelling dislocation dynamics, passage from atomistic to continuum, dynamical aspects of microstructures, transport equations, homogenisation for dynamical problems, atomistic and multiple scale computations. However, the participants listed further emerging topics which one might want to address in a future, possibly larger, workshop: dynamics at nonzero temperature, quantum analysis of microstructural state variables, higher order phase transitions, reversible and irreversible processes, a stronger emphasis of computational methods and high-fidelity modelling. Of course, the topics and techniques discussed at the workshop continue to be active fields of research and will be developed and be refined. The field of mathematical materials science and in particular discrete-to-continuum problems will require the development of new mathematical tools (e.g., building on Wigner and defect measures).

Contact between participants. The workshop offered the opportunity to in-depth, high-level interactions across traditional disciplinary boundaries. There were intense discussions during and after the talks, which continued beyond the official closure of the conference on noon at Friday at least until the ICMS closed after 6pm. It is almost certain that new collaborations will emerge from this. For example, some mathematicians and engineers met at the ICMS for the first time and now plan to work on a model for shear bands and its mathematical analysis. It is most likely that other collaborations will emerge as well. One participant mentioned that a discussion at the ICMS helped him to solve one important

technical problem in his recent work. Some surprising possible new connections were found, for example a potential link between wiggly energies and hysteresis operators as presented by Visintin.

Mix of participants. We did receive several favourable comments by the participants, describing the diversity and interdisciplinarity of the audience and the specific topics as a "source of inspiration". There were some concerns that the workshop, with a focus on modern mathematical techniques, might be less rewarding for participants with a background in Engineering. However, we were pleased to learn that the contrary was the case. For example, one Professor of Mechanics described the workshop as "among the very best workshops I have attended. The stimulating discussions during and after the talks were truly terrific".

Some young participants were invited on short notice. Reluctantly, we offered them the possibility to present their work. Among them was a PhD student from the UK. We were pleased to learn that he has subsequently been invited to visit another participant of the workshop in the UK. As a result of regular and last-minute invitations and walk-ins, slightly more than 10% of the participants were local to Edinburgh.

Germany was strongly represented. This is partially a consequence this country's particular strength in this field, which in turn can be partially traced back to funding by the DFG German Priority Programme *Analysis, Modeling and Simulation of Multiscale Problems*.

We made the deliberate decision to keep the workshop relatively small, despite warnings that there will be a significant interest in the workshop and consequently pressure from potential participants. In the end, we decided to turn down some potential participants, and have not invited some eminent researchers who might have made the conference even more rewarding. Given the size of the ICMS, this was probably the right decision, as the lecture hall was almost full.

Organisational issues. The organisation of the workshop went very smoothly, which is mainly due to the very efficient and friendly help of Tracey Dart and Morag Burton.

The participants also praised the friendly and helpful personnel. The only criticisms were about the speed of the Internet access and some participants felt that the distance between the conference venue and Pollock House respectively MacKenzie apartments were large.

As organisers, we felt that Maxwell's birthplace is a lovely and stimulating location, but it is also limited as far as space is concerned. The limited size of the conference has its pluses and minuses. We would have liked to invite a slightly larger number of eminent specialists in the field. However, the limited size made the workshop very intense and focused. What we lacked definitely in this workshop were one or two additional breakout rooms. Again, the intimate atmosphere of 14 India Street on the other hand was mentioned by the participants to be one of the reasons of the success of the workshop.