EUROPEAN MECHANICS SOCIETY

Colloquium Final Report

N. 636 – Modulation of physico-chemical processes by elastic strain engineering

Dates and location: **22/05/2023 - 24/05/2023, Besançon, France**

Chairperson **Fabien AMIOT**

Co-Chairperson **Javier LLORCA**

Conference fees

- Early-bird registration **260.0 €**
- Late registration **360.0 €**

What other funding was obtained? **We also received funding from Région Bourgogne-Franche Comté, Besançon City and Mecamat association.**

What were the participants offered? **The participants were offered 2 lunches, 1 dinner and two daily coffee breaks.**

Number of members of Euromech (reduced registration fee) **10**

Number of non-members of Euromech (full registration fee) **10**

Applicants (members)

- Fabien Amiot
- Kirill Bolotin
- Artur Braun
- Long-Qing Chen
- Francisco Guinea
- Hosni Idrissi
- Ju Li
- Javier LLorca
- Darrell Schlom
- Jorg Weissmuller

Applicants (non members)

- Yves BELLOUARD
- Qing Chen
- Gaël Chevallier
- Benjamin Davidovitch
- Ho-Nyung Lee

- Samuel Manas-Valero
- Javier Martín-Sánchez
- Carmen Martínez Alonso
- Yong Xie
- Robert Young

Scientific Report

Large elastic deformations modify the electronic structure of materials, leading to changes of their physical and chemical properties, which can even be tuned as a function of the applied strain tensor. The concept of elastic strain engineering is not new and has been successfully applied to enhance the electron and hole mobility in complementary metal-oxide semiconductors, to transform paramagnetic into ferromagnetic ones, or to increase the catalytic activity of metals. In general, the effect of elastic deformations on the physical and chemical properties of materials becomes relevant when elastic strain levels ? 1-2% are reached. These strains levels can only be achieved, however, under conditions of hydrostatic pressure in bulk solids because tensile or shear elastic deformations are relaxed for values < 1% due to the nucleation of defects (dislocations, fracture). Nevertheless, large elastic deformations in traction or shear (which can reach values close to the theoretical limit of 10%) can be achieved nowadays in different types of nanomaterials (nanowires, two-dimensional materials), thin films or bulk materials with an architectured microstructure. This holds true whatever the materials class, and metals, ceramic or organic materials may be considered.

The possibility to apply large elastic strains provides a way to tailor the physico-chemical properties of materials (electronic, optical, magnetic, catalytic, etc.) by systematically varying the 6 components of the elastic strain tensor, opening a huge field to develop new functional materials with optimal properties for specific applications. The topic is interdisciplinary because it lies at the intersection among mechanics, physics, chemistry, materials science and surface science. It moreover involves fundamental theoretical analyses of the mechano-chemical coupling as well as state-of-the-art processing and in-situ characterization techniques to manufacture highly strained materials and measure their multi-physical properties.

The colloquium on “Modulation of physico-chemical processes by elastic strain engineering” was thought as an interdisciplinary discussion forum among scientists with different backgrounds and expertise to analyze the current status and the perspective of elastic strain engineering. There were 21 participants and 18 presentations. Ample slots were allocated for the talks, so that a lot of exciting discussions arose during the presentations and during lunches or coffee breaks. Specific topics addressed in the talks and discussed included :

• Modeling of coupled phenomena using first principles and continuum mechanics tools :

Two distinct families of coupled phenomena have been addressed when focusing on modeling issues. On one hand, ferroelectric thin film and heterostructures have been considered. These have been used to demonstrate that coherent and incoherent strain phase diagrams may be extremely powerful tools to guide the strain tuning of these ferroelectric materials. These diagrams are analog to the better-known temperature-composition phase diagrams. They can be refined using a phase field method to include the coherency strain energy, so that the combination of phase field and thermodynamical stability analysis to model the response of multifunctional structures.

On the other hand, the coupling between chemistry or electrochemistry and mechanics at interfaces can be strong and is exploited in novel materials concepts that afford unexpected functional behavior. In particular, metal/water hybrid nanomaterials that behave similar to piezoelectric ceramics exemplify this concept. With regard to bulk phenomena, interstitial solid solutions containing mobile solute provide a test bed for theories of chemo-mechanical coupling. When mobile solute atoms are inserted, for instance hydrogen into palladium, the elastic response of hybrid nanomaterials switches from the conventional, constant-composition response to open-system elasticity. This affords a verification of the theory of open-system elastic behavior, and it can be the basis of nanomaterials with tunable elastic stiffness.

Alternatively, micro-cantilever based systems offer another convenient system to implement couplings between chemistry or electrochemistry and mechanics at interfaces. These open systems allow for the implementation of various imaging techniques, so that refined theories (and in particular higher-grade elasticity) can be probed at the very local scale. These simple geometries also allow to derive simple mechanical solutions, even for complex coupling phenomena such as elasto-capillarity. Specific arrangements displaying non intuitive behaviors can thus be devised.

• Experimental techniques to induce large elastic strains and monitor multi-physical properties in nanostructured materials, thin films and materials with low dimensionality

Several methods aimed at imposing large strains have been discussed. In order to strain thin films, a first route consist in straining the substrate, before releasing the corresponding strain energy. Different approaches to initially strain the substrate may be considered. A versatile lab-on-chip test platform, which allows to probe couplings, was presented. Another approach consists in exploiting fs laser pulses to locally modify the underlying substrate. Alternatively, it has been shown that oxide thin films could be elastically strained by several percent using substrates with appropriate structural motifs.

The superior strain limits of 2D materials, such as graphene and MoS2 , make them of special interest
for strain engineering. However, several challenges remain, including a lack of an easy straining methodology. Multiple solutions to these challenges, pushing classical approaches to the limit, have been presented and discussed. Van der Waals heterostructures exploiting a spin cross-over have also been shown to be a promising route to control the strain in 2D materials.

Measuring the imposed strain also proved to be challenging with 2D materials, and several possible approaches have been discussed. If Raman spectroscopy proved to be an efficient route to measure strains in cracked graphene single crystals, the periodic character of these 2D materials also allows to exploit moiré patterns.

• Tailoring of material properties (catalytic, corrosion, optical, magnetic, phononic, electronic and optoelectronic properties, etc.) for applications by means of elastic strain engineering

Besides the well-known uses of strain to tailor physico-chemical properties, emerging applications have been identified and presented. In particular, strain has been shown to control the emission properties of single photon sources, making mechanical quantities at the heart of quantum information processing. This is further demonstrated by the use of non-uniform strain fields to transport excitons, whose valley lifetime and coherence may furthermore be controlled by strain.

Last but not least, methodologies for the computational design of optimal material-strain couples based on first principles assisted by machine learning have been extensively discussed. A particularly striking example, demonstrating the use of density functional theory simulations and a decision tree regression model to identify a abundant and cheap alternative to platinum as catalyst in electrolytic hydrogen production, finally highlighted the key role of elastic strain engineering in future technologies.

Number of participants from each country

COUNTRY	PARTICIPANTS
Belgium	1
Spain	6
Switzerland	3
United States	5
United Kingdom	1
France	2
Germany	2
TOTAL	**20**

Please send this report in electronic form to the Secretary General of EUROMECH, within one month after your Colloquium.