12 months post-doc position:

Experimental investigation of the effect of mechanical stress on the lithiation of amorphous silicon

General features of the position:

- Mainly experimental work.
- Multiphysics problem at the interface between mechanics and electro-chemistry.
- Part of a collaboration between the **solid mechanics laboratory (LMS)** and the **condensed-matter physics laboratory (LPMC)** of Ecole polytechnique.

Scientific context and objectives:

Amorphous silicon (a-Si) is viewed as a promising material for the anode of **lithium-ion batteries (LIB)** as it offers a theoretical capacity (density of energy per unit mass) ten times higher than that of graphite, the material currently used as anodes of commercial LIBs. When lithiated and delithiatied, a-Si shows large mechanical deformations (volume change of 300%), experiences stresses of the order of the GPa, and suffers fracture after a few charge-discharge cycles. These different features indicate a strong coupling between the **electro-chemistry** involved in the lithiation of silicon and its **state of mechanical stress**. (Zhao 2019)

In particular, theoretical models developed over the last decade predict a significant effect of the mechanical stress on the process of lithiation, which shall reflect in a **stress-induced change of the lithiation potential** (Bower 2015). Existing experimental works suggest that such a stress-potential coupling exists, although it has only be investigated indirectly. (Sethuraman 2010)

The objective of this work is to demonstrate and quantify experimentally the effect of stress on the lithiation potential by exerting in situ mechanical stress on a-Si silicon during the lithiation process.

Concretely, our team presently has a working set-up for the lithiation of a-Si thin-film. This consists of the deposition through PECVD of a-Si thin films on steel plates and their lithiation in a home-made cell. (Feng 2019) The present work aims at carrying out lithiation under varying levels of stress by inserting the lithiation cell in a tensile machine (see, e.g., (Guin 2020) for such a coupled experiment on the different problem of solar cells).

To this end, we envisage the completion of the following tasks

- Performing preliminary tests to validate the tightness of the lithiation cell (filled with liquid electrolyte) when the substrate is subject to mechanical stress. Identify the adequate tightening of the system.

- Characterize the strain experienced by the working area of the steel substrate (where the a-Si is deposited) when the latter is subject to tensile strain in the presence of the lithiation cell.
- Design and carry out coupled experiments where the a-Si is lithiated under different levels of stress in order to characterize the stress-potential coupling. Experiments will be possibly carried out under multiaxial loading.

Candidate:

The candidate will be a young doctor with experience in **experimental mechanics** and interest for multiphysics systems (e.g., with a taste for acquiring new experimental skills related to electro-chemistry).

Supervision:

The post-doc is supervised by Laurent Guin (Assistant Professor at Ecole polytechnique and member of the LMS) in collaboration with Michel Rosso and François Ozanam (CNRS research scientists at LPMC).

Workplace:

The work will take place at the laboratory LMS on the campus of Ecole polytechnique in close collaboration with the laboratory LPMC (same building as LMS).

Salary:

The employer is Armines and the salary will depend on the experience of the candidate, a least 2780 € gross per month (approximately 2085 € net salary).

Starting date and duration:

The post-doc position shall start between January and April 2022 and is funded for 12 months.

How to apply:

Please send an e-mail to laurent.guin@polytechnique.edu with a curriculum vitae.

1 References

Bower, A. F., Guduru, P. R., & Chason, E. 2015. «Analytical solutions for composition and stress in spherical elastic–plastic lithium-ion electrode particles containing a propagating phase boundary.» *International Journal of Solids and Structures* 69: 328-342.

Feng, Y., Panagopoulou, M., Cheriet, A., Koo, B. M., Henry-de-Villeneuve, C., Rosso, M., & Ozanam, F. 2019. «Lithiation of pure and methylated amorphous silicon: Monitoring by operando optical microscopy and ex situ atomic force microscopy.» *Electrochimica Acta* 302: 249-258.

Guin, L., i Cabarrocas, P. R., Jabbour, M. E., & Triantafyllidis, N. 2020. «Effect of strain on the dark current-voltage characteristic of silicon heterojunction solar cells.» *Solar Energy* 196: 457-461.

Sethuraman, V. A., Srinivasan, V., Bower, A. F., & Guduru, P. R. 2010. «In situ measurements of stress-potential coupling in lithiated silicon.» *Journal of the Electrochemical Society* 157(11): A1253.

Zhao, Y., Stein, P., Bai, Y., Al-Siraj, M., Yang, Y., & Xu, B. X. 2019. «A review on modeling of electro-chemo-mechanics in lithium-ion batteries.» *Journal of Power Sources* 413: 259-283.