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A FINITE ELEMENT MODEL FOR DIFFUSION-INDUCED FRACTURE IN DUAL GRAPHITE BATTERY ELECTRODES

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Electrochemical energy storage is called to play an important role as a complement to renewable energy harvesters such as photovoltaic panels or wind turbines, and overcome the limitations derived from their availability. Traditional Li-ion batteries (LIBs) can manage efficiently this storage, but rely on the use of scarce and non-recycled materials. An interesting alternative are Dual Graphite Batteries (DGB), which arise as a promising, sustainable, and economic alternative to LIBs due to the use of abundant and recyclable materials [1]. However, nowadays DGB still present some technical limitations. In particular, during battery operation the intercalation and deintercalation of ions into the graphite electrodes cause huge volume changes and stresses in the host material, which can eventually lead to micro-cracks. These cracks isolate the electrode particles, threaten the electrical conductivity and generate new surfaces where solid electrolyte interface can grow. For this reason, it is of great importance to understand this degradation mechanism which limits the performance and durability of the battery.

In this work, we propose a finite element (FE) model to analyse the mechanical degradation in the microstructure of DGB electrodes. Namely, we propose a thermodynamically consistent approach, considering stress-diffusion coupling within a finite deformation framework combined with a phase-field model for fracture. To represent the brittle, disordered material behavior of graphite, we use a Weibull distribution for the elastic modulus and fracture energy within the Saint-Venant Kirchhoff constitutive model. The diffusion in the host electrode depends on the chemical potential and the phase-field damage model follows the hybrid approach by Ambati et Al. [2].

The model has been implemented in the FE-code FEniCS, which is used to study the mechanical degradation in DGB electrodes. This model reveals the crack nucleation and propagation in actual graphite DGB microstructures, which can be obtained from environmental scanning electron microscopy (ESEM) or a recently-develop virtual microstructure generator. Understanding this phenomenon may help the virtual design of DGB with improved properties.

REFERENCES

[1] Beltrop, K. and Beuker, S. and Heckmann, A. and Winter, M. and Placke, T., Alternative electrochemical energy storage: potassium-based dual-graphite batteries. *Energy Environ. Sci.* Vol. **10**, 2017.

[2] Ambati, M., Gerasimov, T., De Lorenzis, L., A review on phase-field models of brittle fracture and a new fast hybrid formulation. *Comput Mech.* Vol. **55**, 2015.