Bending impact on the performance of a flexible Li$_4$Ti$_5$O$_{12}$-based all-solid-state thin film battery

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Supporting Information
Figure S1: Charge and discharge cycles for the flexible all-solid-state battery at different C-rates for different bending states.
Figure S2: AFM measurements done on a) bare flexible ceramic substrate, b) Flexible ceramic substrate + 200 nm LTO layer, c) bare SiOx substrate and d) SiOx substrate + 200 nm LTO layer.
Figure S3: Cross section SEM of full battery stack on a) a flexible ceramic substrate and b) a rigid SiOx/Si substrate.
Calculation procedure to define Figure 4

Layer thicknesses and values:

Flexible substrate: 40 µm
Ti adhesion layer: 20 nm
Pt current collector: 70 nm
Li$_4$Ti$_5$O$_{12}$ cathode electrode: 200 nm
LiPON solid electrolyte: 500 nm
LiFePO$_4$ anode electrode: 1 µm
Total thickness: 41.79 µm

Mechanical Neutral Plane situated at: 20.895 µm
(d) Li$_4$Ti$_5$O$_{12}$ electrode distance to neutral plane: 19.295 µm
(E) Young’s Modulus: 200 GPa
(Rc) Bending radii: 25, 17 and 14 mm

The stress for each bending radius is calculated by:

$$\sigma = \frac{E \cdot d}{Rc}$$

Resulting in:

$$\sigma = 154, 227 \text{ and } 276 \text{ MPa for } Rc = 25, 17 \text{ and } 14 \text{ mm, respectively.}$$

The force applied at each bending state is considered following the relation:

$$F = \sigma \cdot A$$

where A is the cross-sectional area of the active materials in the flexible battery

$$A = 36 \text{ mm} \times 41.79 \text{ µm} = 1.5044 \times 10^{-6} \text{ m}^2$$

Giving as a result for the Force as:

$$F = 232, 341 \text{ and } 415 \text{ Newtons for } Rc = 25, 17 \text{ and } 14 \text{ mm, respectively.}$$

The value for strain can be defined with the strain to stress relation:

$$\varepsilon = \frac{\sigma}{E}$$

Resulting in values of strain of:

$$\varepsilon = 0.000772, 0.00114 \text{ and } 0.00138 \text{ for } Rc = 25, 17 \text{ and } 14 \text{ mm, respectively.}$$

This values are plotted in Figure 4 and are related to the corresponding capacity changes for each bending radius depicted in average values from Table 1. To link it to the results from
Ning et al.\textsuperscript{14} the maximum strain limit is calculated according to the specifications provided by the supplier from the Weibull distribution obtained from the physical and mechanical properties from https://www.enrg-inc.com/technology.

![Weibull Distribution](https://www.enrg-inc.com/technology)

This is calculated by assuming a Young’s modulus ($E$) of 200 GPa which is defined for the flexible ceramic substrate and by considering a failure probability of 98 % obtained when applying a strength of 1.2 GPa. Using the cross sectional area ($A$) of 0.8E-6 m$^2$. The force obtained at 1.2GPa strength by the relation $F = \sigma A$, results in: 96 Newtons. When applying this same force in the geometry of our thin film flexible battery ($A = 1.5044E-6$ m$^2$) the resulted stress achieved is $\sigma = 638$ MPa. Next, the value for strain can be defined with the strain to stress relation ($\varepsilon = \sigma/E$) resulting in a maximum strain $\varepsilon = 0.003$. This value is linked to the 5 % maximum lattice strain from Ning et al.\textsuperscript{[14]} It is assumed that the maximum capacity change is 5.47 % (Table 1) for both conditions of bending. That is, a maximum change of ± 5.47 % linked to the Lithium diffusion energy barrier of 1 eV and to a free Lithium diffusion pathway (Energy barrier = 0). In addition, it is assumed that under zero strain the capacity the change in capacity is 0.