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Highlights

Surface strain on prismatic Li-ion cells: thermo-mechanical modelling, calibration and validation with gauges

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- The model differentiates strain due to lithium intercalation from thermal effects
- The model is calibrated by running two cycling tests at low and moderate C-rates
- Calibrated model simulation and strain gauge measurement agree for a high C-rate

Surface strain on prismatic Li-ion cells: thermo-mechanical modelling, calibration and validation with gauges

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Abstract

This paper proposes a 0D thermo-mechanical model of the surface strain, measured locally by a gauge bonded to the casing of a prismatic Li-ion cell. The simplicity of this model makes it suitable for in operando diagnostic. Three contributions are identified in the modelling: i) casing deformation due to Li intercalation as a function of charge state or lithiation rate, ii) casing thermal expansion that cannot be fully compensated for, even when two gauges are used in a Wheatstone bridge, iii) casing deformation due to jellyroll thermal expansion. At low C-rate, an overall thermal expansion coefficient can describe both thermal effects. At high C-rate, a transient thermal model is required, to describe both irreversible losses and reversible entropic heat. Experimental validation was carried out with commercial 29 Ah Graphite/NMC prismatic cells. Model parameters and intrinsic characteristics (strain due to Li intercalation and reversible entropic heat) were estimated from strain tests performed at C/10 and C/5 rates. The accuracy of the model was then proven by charge and discharge tests carried out at 1C rate.

Keywords: Li ion cell, strain gauge, thermo-mechanical modelling, lithium

1. Introduction

Lithium-ion batteries are increasingly part of our lives, as this technology is an essential solution for electrical energy storage. One of the challenges in terms of sustainability is to extend the life of Li-ion cells as far as possible, which requires effective in operando diagnostics. Electrical measurements, i.e. voltage and current, are generally used to perform the diagnostic of Li-ion cells. For a sake of illustration, estimation of SoC (State of Charge) relies on a direct measurements such as OCV (Open Circuit Voltage), AC impedance, current pulse measurements or coulomb counting [1]. Temperature is also monitored to manage battery state, durability and thermal stability [2, 3, 4].

Monitoring other physical quantities, such as the mechanical behaviour, can be of interest to improve these diagnostics. It is well known that a Li-ion cell swells during a charge/discharge cycle due to the intercalation of Li ions within the electrode materials. In particular, a volume change of more than 10% can be achieved in a graphite electrode [5]. Volume changes of Li-ion cell can be measured using a wide range of techniques, including displacement sensors [6], load cells [7], optical fiber sensors [8] or computed tomography [9, 10]. However, one of the most attractive technical solutions for onboard applications are strain gauges, which provide simple and low-cost measurement. Recently, Beznosov et al. have shown that strain ϵ recorded with gauges can be experimentally used to perform a differential strain analysis $d\epsilon/dV$ in a similar way to the well-known differential capacity analysis dQ/dV [11].

However, it is necessary to develop a simple physical model in order to exploit the measurements performed with strain gauges for onboard applications. On this point, there is a lack of literature. Electrochemical-thermal-mechanical models have been proposed on the basis of the pseudo-2D approach [12, 13]; but these models require a large number of parameters, which is prohibitive for an onboard application. Other authors have proposed phenomenological models that successfully predict experimental data [14] but are unable to interpret the results, making them unusable for advanced diagnostics such as the differential strain analysis mentioned previously. Finally, data-driven models can also be implemented. In [15], authors used strain data to estimate the depth of discharge. The success of this approach proves that there is relevant information in the strain measurement, but as with the phenomenological approaches, data driven models cannot be used for further physical analysis.

This paper proposes a model of the surface strain measured locally by a gauge bonded to the casing of a prismatic cell. On one hand, the model helps identifying the strain due to the intercalation of Li ions in the electrodes. On the other hand, the model takes into account to thermal effects: the thermal expansion of the jellyroll which causes mechanical deformation of the casing and the thermal expansion of the casing itself; the latter cannot be fully compensated for, even when two gauges are used in a Wheatstone bridge. A steady state thermal model is introduced for low C-rate, leading to an overall thermal expansion coefficient of the two thermal phenomena. A transient thermal model is required for high C-rate, where internal heat sources have to be described.

Section 2 gives details of the experimental setup for measuring strain during charge/discharge; a technique is proposed to suppress a slow perturbation signal, mainly visible at low C-rate. The modelling is presented in section 3 in the cases of low and high C-rates. Section 4 presents the various experimental testing performed to calibrate and validate the model. First, the strain due to Li intercalation is estimated from a C/10 measurement, and the overall expansion coefficient, valid for low C-rates, is determined. Next, the reversible entropic heat is estimated using a C/5 test and the coefficient due to casing expansion is determined. Finally, the complete model is built: a simulation is carried out at 1C rate and compared with measurement performed at the same C-rate.

2. Experimental setup

2.1. Cell cycling

A NMC-rich Samsung 29Ah prismatic Li-ion cell was used in the experiment. No precise information is available about the materials used for the electrodes; the cathode is assumed to be NMC622 and the anode graphite.

For each C-rate, the cycle test follows the same pattern. First, a CC-CV charge is performed with an end-of-charge voltage set at 4.15V. This is followed by a relaxation time of 3 hours. Next, a CC discharge is carried out until a voltage of 2.7 V is reached. Finally, the cycle ends with a relaxation time of 3 hours.

The cell was placed on a support without mechanical fastenings to allow free swelling.

A thermocouple was placed in contact to the casing to measure the surface temperature and another thermocouple was placed in the enclosure to measure the ambient temperature.

2.2. Strain measurements

Two strain gauges are used to measure casing strain as detailed in Fig. 1. The first gauge is glued to the surface of the casing at the center of its largest area; the other gauge is placed in contact with the cell casing to compensate for thermal effects.

Figure 1: Experimental setup with two strain gauges

The two gauges are mounted in a Wheatstone bridge, from which a voltage is measured. After amplification, this voltage is given by [16]:

$$V_{gauge} = \frac{1}{4}V_{bridge}G_aG_g\epsilon_{gauge} \quad (1)$$

where V_{bridge} is the supply voltage of the bridge, G_a the amplifier gain, G_g the gauge gain and ϵ_{gauge} the in-plane strain.

Gauges CEA-13-250UWA-350 were used in the experiments: the gauge gain G_g is 2.1 and its resistance 350 Ω . Voltage V_{bridge} was set at 5V in order to obtain a sufficient signal-to-noise ratio while limiting the Joule heat generated by the gauges (20 mW on a grill surface of 5 mm²). The amplifier gain G_a was set to 1000.

Measurements were carried out with a 29 Ah prismatic cell subjected to several charge/discharge cycles at different C-rate. However, in none of the tests was the measured gauge voltage perfectly periodic: a signal with very

slow dynamics overlaps with the expected periodic pattern. This effect is particularly noticeable at C/10 rate (see Fig. 2), less significant at higher C-rate because the cycle duration is shorter.

Figure 2: Gauge and cell voltages as well as ambient temperature measured for cycling performed at C/10 rate

The gauge captures strain induced by small external stresses, such as small vibrations due to the use of an enclosure equipped with a high power compressor. To avoid vibrations, the experiments were carried out in the non-ventilated enclosure, which explains the small variations in ambient temperature observed in Fig. 2. However, it remains a perturbation signal that can nevertheless be removed as described in section 2.3, in contrast to the intermittent perturbation signal generated by vibrations when the enclosure is ventilated.

It should be noted that other authors have also observed that strain gauge measurements were not perfectly periodic when the cell undergoes cycles of charge/discharge [7, 11]. The transient regime may last several days. This phenomenon is probably due to relaxation caused by the viscosity of cell materials.

2.3. Correction of the non-periodic perturbation

The observed slow signal is assumed to add to the expected periodic pattern:

$$V_{gauge}(t) = \sum_k V_{pattern}(t - kT_{cycle}) + V_{perturbation}(t) + V_{noise}(t) \quad (2)$$

where $V_{pattern}$ is the periodic pattern defined on a period $[0, T_{cycle}[$, $V_{perturbation}$ the slow perturbation signal and V_{noise} the measurement noise.

A 5-th order polynomial is introduced to fit the signal $V_{perturbation}(t)$. In addition, 4 measurement points are chosen during a cycle (beginning and end of charge as well as beginning and end of discharge), giving a total of 20 measurement points over the 5 periods selected. Using least squares, the 6 polynomial coefficients are computed, as well as the values V_{p1} , V_{p2} , V_{p3} and V_{p4} of the periodic pattern $V_{pattern}$ for the 4 points selected over a period.

The signal $V_{perturbation}(t)$ obtained is plotted in Fig. 3 (curve in red) in the case of the experiment at C/10 rate shown in Fig. 2. By subtracting $V_{perturbation}(t)$ from the original gauge voltage $V_{gauge}(t)$, the repetitive pattern $V_{corrected}(t)$ is extracted, as shown in Fig. 3 (curve in black).

Figure 3: Gauge voltage and correction obtained after identification of the slow perturbation signal at C/10 rate.

For the experiment at C/5 rate, the slow perturbation $V_{perturbation}$ affects the measured gauge voltage less, since cycling is twice as fast. An affine function is sufficient to fit $V_{perturbation}(t)$ for an interval restricted to one cycle period: the two coefficients of the linear function are chosen so that the value of signal $V_{corrected}$ at the beginning of the cycle is the same as the value obtained at the end of the cycle.

The same procedure as the one used at C/5 rate was applied to extract the periodic strain pattern at 1C rate. For the 1C rate test, the effect of $V_{perturbation}$ is almost negligible: the difference is only 8 mV between the gauge voltage measured at a given instant for two successive cycles, while the total variation is 140 mV over a cycle.

3. Modelling of surface strain

3.1. Strain due to the lithiation and thermal effects

Once the perturbation signal described in section 2.3 has been removed, strain $\epsilon_{pattern}$ induced by cycling phenomena can be calculated using the relationship between voltage and strain given by Eq. (1). Strain $\epsilon_{pattern}$ is the result of two effects: i) mechanical strain ϵ_m due to internal forces acting on the casing, ii) in-plane thermal expansion of the casing, which is not fully compensated for by the two-gauge device [17].

$$\epsilon_{pattern} = \epsilon_m + \alpha_{c-g}(T_s - T_0) \quad (3)$$

where α_{c-g} is the difference of thermal expansion coefficients between the casing and the gauge, T_s the surface temperature and T_0 the initial temperature.

In Eq. (3), the mechanical strain part ϵ_m contains two contributions: i) the mechanical deformation of the casing caused by the change in volume due to Li intercalation in the electrodes; it is referred as ϵ_{Li} ii) the mechanical deformation of the casing caused by the change in volume of the jellyroll due to thermal expansion; it is referred as $\epsilon_{\Delta L_z}$.

$$\epsilon_m = \epsilon_{Li}(SoC) + \epsilon_{\Delta L_z}(T) \quad (4)$$

The characteristic ϵ_{Li} as a function of SoC or lithiation rate can be obtained experimentally via a low C-rate test, where thermal effects are not significant. This experiment is presented in section 4.1.

To describe the jellyroll volume change due to thermal expansion, it is necessary to introduce a thermal model. In this paper, a 1D model is used to

describe the temperature distribution in the jellyroll thickness, from which the total out-of-plane stretch ΔL_z due to thermal expansion can be deduced in the absence of casing. The in-plane strain $\epsilon_{\Delta L_z}$ induced in the presence of the casing is considered to be proportional to ΔL_z . This assumption is correct when materials have linear mechanical properties as proved in Appendix A. In addition, when a low C-rate is assumed, a steady state model can be considered and an equivalent thermal expansion coefficient $\alpha_{\Delta L_z}$ can be defined for the in-plane strain, as shown in section 3.2. When a high C-rate is assumed, the heat generated by the cell needs to be modelled in more detail, describing irreversible losses and reversible entropy heat as shown in section 3.3.

3.2. Low C-rate case

As mentioned previously, strain due to thermal effects takes two distinct forms: i) in-plane thermal expansion of the casing, that is partially compensated for by the second gauge placed in contact with the casing ii) thermal expansion of the jellyroll which induces forces on the casing, leading to mechanical deformation.

To take this a step further, a 1D thermal model is introduced, in which the Oz axis is considered in the out-of-plane direction, with the origin taken at the middle of the cell thickness (see Fig. 1). In addition, the heating power \dot{Q} induced by the cell is considered to be uniformly distributed throughout the cell volume. Finally, the temperature distribution T is assumed to be governed by the steady state heat equation [18]:

$$k \frac{d^2 T}{dz^2} + \frac{\dot{Q}}{V} = 0 \quad \text{with} \quad \left. \frac{dT}{dz} \right|_{z=0} = 0$$

$$-k \left. \frac{dT}{dz} \right|_{z=L_z/2} = h(T_s - T_0) \quad (5)$$

where k is the effective thermal conductivity of the cell, h the global heat transfer coefficient between the cell and half of its environment, L_z the cell thickness and V the cell volume.

The solution of Eq. (5) is:

$$T(z) = \frac{h}{L_z k} (T_s - T_0) \left(\left(\frac{L_z}{2} \right)^2 - z^2 \right) + T_s \quad (6)$$

In the absence of casing, this temperature distribution would generate an out-of-plane thermal expansion, expressed as follows:

$$\Delta L_z = 2 \int_0^{L_z/2} \alpha (T(z) - T_0) dz = \alpha L_z \left(1 + \frac{h L_z}{6k} \right) (T_s - T_0) \quad (7)$$

where α is the homogenized coefficient of thermal expansion (the jellyroll is made up of successive thin layers of positive electrode, separator and negative electrode materials).

The presence of the casing constrains the cell swelling. The resulting in-plane strain $\epsilon_{\Delta L_z}$ is assumed to be proportional to ΔL_z (see Appendix A for details); in particular, a coefficient γ is introduced to express this proportionality.

Finally, the total strain is the sum of the strain due to lithiation, strain due to jellyroll thermal expansion and strain due to casing thermal expansion:

$$\epsilon_{pattern} = \epsilon_{Li} + \alpha_{\Delta L_z} (T_s - T_0) + \alpha_{c-g} (T_s - T_0) \quad (8)$$

with the thermal expansion coefficient $\alpha_{\Delta L_z} = \gamma \alpha L_z (1 + h L_z / 6k)$.

Introducing the total thermal expansion coefficient $\alpha_{cell} = \alpha_{\Delta L_z} + \alpha_{c-g}$ in Eq. 8 gives:

$$\epsilon_{pattern} = \epsilon_{Li} + \alpha_{cell} (T_s - T_0) \quad (9)$$

3.3. High C-rate case

For the thermal model, steady state regime is no longer considered. The heat equation is then given by [18]:

$$k \frac{\partial^2 T}{\partial z^2} + \frac{\dot{Q}}{V} = \frac{C_{th}}{V} \frac{\partial T}{\partial t} \quad \text{with} \quad \left. \frac{\partial T}{\partial z} \right|_{z=0} = 0$$

$$-k \left. \frac{\partial T}{\partial z} \right|_{z=L_z/2} = h (T_s - T_0) \quad (10)$$

where C_{th} is the cell thermal capacity.

In the absence of casing, the temperature distribution would generate an out-of-plane thermal expansion, expressed as follows (see Appendix B for details):

$$\Delta L_z(t) = \frac{\alpha L_z}{C_{th}} \int_0^t \left(\dot{Q} - 2h S_{xy} (T_s - T_0) \right) dt \quad (11)$$

with S_{xy} the largest lateral surface of the casing.

The in-plane strain due to out-of-plane thermal expansion of the jellyroll can then be obtained by applying the same factor γ as that introduced in the low C-rate problem modelling. Finally, the total strain $\epsilon_{pattern}$ is given by:

$$\epsilon_{pattern} = \epsilon_{Li} + \frac{\alpha'_{\Delta L_z}}{C_{th}} \int_0^t \left(\dot{Q} - 2h S_{xy} (T_s - T_0) \right) dt + \alpha_{c-g} (T_s - T_0) \quad (12)$$

with the thermal expansion coefficient $\alpha'_{\Delta L_z} = \gamma \alpha L_z$.

The source \dot{Q} is due to irreversible and reversible heat inside the cell [19]:

$$\dot{Q} = (V_{cell} - OCV) I + TI \frac{dOCV}{dT} \quad (13)$$

where V_{cell} is the load cell voltage, I the load current and T the temperature.

The term $dOCV/dT$ can be extracted experimentally from strain measurement at a moderate C-rate test. This experiment is presented in section 4.2.

4. Experimental results and discussion

4.1. Estimation of the characteristic ϵ_{Li}

A measurement at C/10 rate has been performed to extract the strain due to the Li intercalation. As presented in the section 2.3, the gauge voltage measurement at C/10 rate has been corrected to extract the periodic pattern. Instead of describing the strain $\epsilon_{pattern}$ as a function of time, it is more suitable to display it as a function of the lithiation rate at the negative electrode, where the largest volume variation is expected during a cycle [15].

To convert the amount of charge into the proportion of lithium in the negative electrode, an OCV model of the cell was built from the OCPs (Open Circuit Potentials) of the two electrodes. Specifically, the pseudo OCV, experimentally estimated by averaging the cell voltage in charge and discharge at C/10 rate, was fitted using the theoretical OCPs, NMC622 for the cathode and graphite for the anode.

Fig. 4a shows the strain measured after correction as a function of the anode lithiation rate. The strain is different between charge and discharge: this is due to thermal effects, as the temperature varies by more than 1°C during charge or discharge (see Fig. 4b).

Figure 4: (a) Strain obtained after correction of the slow perturbation signal and (b) cell surface temperature measured for a cycle at C/10 rate.

The model built for a low C-rate in section 3.2 was used to extract the characteristic ϵ_{Li} . To justify the steady state assumption considered in section 3.2, the diffusion time in the cell can be calculated using the expression $L_z^2 C_{th}/kV$. Thermal parameters were evaluated by means of a specific experiment in which a thermal resistor was placed on one side of the cell and the temperature rise was measured on each side of the cell in the case of a power step. By analyzing the transient response, the parameters $C_{th} = 1056 \text{ J K}^{-1}$ and $k = 2.94 \text{ W m}^{-1} \text{ K}^{-1}$ were estimated. These values give a diffusion time equal to 512 s i.e. 0.14 h, which is small compared to 10 h, the duration of a charge or discharge.

The strain due to lithiation ϵ_{Li} can be deduced from Eq. (9):

$$\epsilon_{Li} = \epsilon_{pattern} - \alpha_{cell} (T_s - T_0) \quad (14)$$

The thermal coefficient α_{cell} has been chosen so that strains due to lithiation ϵ_{Li} estimated under charge and discharge are as close as possible. Fig. 5a shows the estimated ϵ_{Li} for $\alpha_{cell} = 8 \cdot 10^{-6} \text{ K}^{-1}$. It is worth noting that the evolution ϵ_{Li} as a function of the lithiation rate is close to the graphite volume variation reported in the literature (see Fig. 5b).

To confirm the value of α_{cell} , a test was carried out in the steady state regime with a temperature jump of 5°C for a SoC set at 50 %. As with the cycling tests, this experiment was made difficult by the presence of a perturbation signal. To properly assess this disturbance, the experiment was run over 4 days. The results are reported in the first part of the supplemen-

Figure 5: (a) Strain of the prismatic cell due to Li intercalation extracted at C/10 rate; the interpolation curve was obtained by averaging charge and discharge curves and smoothing the result to reduce noise (b) Theoretical volume change of graphite vs lithium content; data extracted from the supplementary file of [5], also presented in Figure 5c of the same article.

ary file. The total thermal expansion coefficient for a change in ambient temperature is slightly different from that defined for cycling at low C-rate in section 3.2. However, the former coefficient can be deduced from the parameters estimated during the cycling tests and the specific thermal experiment. The value obtained is close to that obtained from the steady state experiment: the difference is around 1%.

A second steady state test was carried out with a SoC jump of 25% at constant temperature. Data processing was more delicate, as the phenomenon of mechanical relaxation is more pronounced than in the constant SoC test with a temperature jump. Nevertheless, the experimental results can be exploited by focusing on a time interval around the SoC change. The results are reported in the second part of the supplementary file. The estimated strain in this steady state test is very close to the result obtained with the cycling test at C/10 rate: the difference is around 4%.

4.2. Estimation of the reversible entropic heat

A measurement at C/5 rate has been performed to extract the heat generated by the cell, and more precisely the reversible entropic heat. Fig. 6a shows the strain $\epsilon_{pattern}$ obtained at C/5 rate after correction of the perturbation signal as described in section 2.3. Strain variation is slightly greater than that obtained at C/10 (approximately 0.004% vs 0.0035%) while tem-

perature variation is considerably greater (about 3.5°C vs 1.5°C, see Fig. 6b).

Figure 6: (a) Strain obtained after correction of the slow perturbation signal and (b) cell surface temperature measured for a cycle at C/5 rate.

The model built for a high C-rate in section 3.3 was used in order to estimate the term $dOCV/dT$ related to the reversible entropic heat.

Extracting the term $dOCV/dT$ requires a few preliminary calculations. First, the strain due to the out-of-plane thermal expansion ΔL_z is isolated from Eqs. (3) and (4):

$$\epsilon_{\Delta L_z} = \epsilon_{pattern} - \epsilon_{Li} - \alpha_{c-g} (T_s - T_0) \quad (15)$$

By inserting Eq. (12) in Eq. (15), one obtains:

$$\frac{d\epsilon_{\Delta L_z}}{dt} = \frac{\alpha'_{\Delta L_z}}{C_{th}} \left(\dot{Q} - 2hS_{xy} (T_s - T_0) \right) \quad (16)$$

Then introducing Eq. (13) in Eq. (16), one finds:

$$\frac{dOCV}{dT} = \frac{1}{T_s I} \left(\frac{C_{th}}{\alpha'_{\Delta L_z}} \frac{d\epsilon_{\Delta L_z}}{dt} + 2hS_{xy} (T_s - T_0) - (V_{cell} - OCV) I \right) \quad (17)$$

where the temperature T in Eq. (13) is chosen equal to the surface temperature T_s because the temperature variation inside the cell is assumed to be small. In the case of the steady state solution (6), a variation of $hL_z/4k \times (T_s - T_0)$ is theoretically expected between the middle and edge temperatures. The parameter h was estimated to 16.3 W K⁻¹ m⁻² for the cell under test. This gives a relative temperature variation between the middle and the edge of the cell of no more than 0.015% for the C/10 rate experiment. Under these conditions, the temperature variation is expected to be moderated for the C/5 rate experiment.

Measured strain $\epsilon_{pattern}$ is given in Fig. 6a and strain ϵ_{Li} has been extracted from measurement at C/10 rate, as shown in Fig. 5a. Surface temperature T_s as well as cell voltage V_{cell} and current I are measured. OCV has already been built using measurements at C/10 rate.

The thermal expansion coefficient $\alpha'_{\Delta L_z}$ introduced in Eq. (12) for a high C-rate is related to the thermal expansion coefficient $\alpha_{\Delta L_z}$ introduced in Eq. (8) for a low C-rate:

$$\alpha'_{\Delta L_z} = \frac{\alpha_{\Delta L_z}}{1 + hL_z/6k} = \frac{\alpha_{cell} - \alpha_{c-g}}{1 + hL_z/6k} \quad (18)$$

Finally, the only unknown in Eq. (17) is the parameter α_{c-g} that gives the difference between the casing thermal expansion coefficient and the gauge one. The coefficient α_{c-g} has been chosen so that the characteristics $dOCV/dT$ estimated under charge and discharge are as close as possible. Fig. 7a shows the estimated $dOCV/dT$ when $\alpha_{c-g} = 2 \cdot 10^{-6} \text{ K}^{-1}$.

Figure 7: (a) Term $dOCV/dT$ during charge and discharge extracted from measurements at C/5 rate; the interpolation curve was obtained by averaging charge and discharge curves and smoothing the result to reduce noise. (b) Term $dOCV/dT$ deduced from the reversible entropic term $\Delta S = FdOCV/dT$ with F the Faraday constant, displayed in Figure 6 of [20]

The evolution $dOCV/dT$ as a function of the lithiation rate is similar to the one reported in the literature (see Fig. 7b). In addition, the $dOCV/dT$ term was estimated from steady state tests following a protocol close to that described in [19]. For a given SoC value, the OCV was measured for different temperature values ranging from 5 to 35°C; the variation in OCV observed enables the value of $dOCV/dT$ to be estimated (see the third part

of the supplementary file). The results obtained for different SoC values are reported in Fig. 7a: the $dOCV/dT$ characteristics obtained from the steady state and the C/5 rate tests are very close.

In addition, the value of thermal expansion coefficient α_{c-g} is realistic. CEA-13-250UWA-350 gauges are partly made of constantan with a thermal expansion coefficient of $14.9 \cdot 10^{-6} \text{ K}^{-1}$. The casing is made of an alloy with a thermal expansion coefficient around $20 \cdot 10^{-6} \text{ K}^{-1}$. Consequently, the value of α_{c-g} is around a few units of 10^{-6} K^{-1} .

4.3. Validation of the model

In order to validate the model, a measurement was carried out at 1C-rate. Fig. 8a shows the strain $\epsilon_{pattern}$ obtained after correction of the perturbation as described in section 2.3. Curiously, there is almost no variation in strain during discharge while it reaches 0.005% during charge. The temperature variation is much greater than in previous cases C/10 and C/5 rates, particularly during discharge where it exceeds 6°C (see Fig. 8b).

Figure 8: (a) and (b) Strain obtained after correction of the slow perturbation signal and cell surface temperature, respectively, measured for a cycle at 1C rate. (c) Comparison between simulation and measurement of the strain during charge and discharge. (d) and (e) Contribution of Li intercalation, casing thermal expansion and jellyroll thermal expansion in the simulation of the strain during respectively charge and discharge

A simulation has been performed at 1C-rate from the model given by Eqs. (12) and (13). The strain ϵ_{Li} is that obtained with the C/10 experiment and the term $dOCV/dT$ is that obtained with the C/5 experiment. The other parameters are the same as those set previously, from the experiments at C/10 and C/5 rates and from the specific thermal experiment (see Table 1).

Parameter	Value
L_z	21 mm
S_{xy}	173 mm \times 85 mm
h	16.3 W m ⁻² K ⁻¹
k	2.9 W m ⁻¹ K ⁻¹
C_{th}	1056 J K ⁻¹
α_{cell}	8 10 ⁻⁶ K ⁻¹
α_{c-g}	2 10 ⁻⁶ K ⁻¹

Table 1: Value of the parameters used in the simulations at different C-rates

Fig. 8c shows a comparison between measurements and simulation. Overall, the model reproduces the strain with an amplitude of about 0.005% as observed during the charge; the model also predicts the small variation of strain measured during the discharge. However, there is a small discrepancy between measurement and simulation. The strain error between measurement and simulation is 14% of the maximum strain value for the charge phase and 16% for the discharge phase.

The model enables to explain the difference in strain observed during charge and discharge as shown in Fig. 8d-e. During charge, the contributions of Li intercalation, casing thermal expansion and jellyroll thermal expansion are additive. During discharge, Li intercalation on the one hand and thermal expansions on the other act inversely.

By assumption, Li intercalation induces the same volume change during charge and discharge. The thermal effect, on the contrary, is different, as shown by the measured surface temperature in Fig. 8b, mainly because

the reversible entropic heat changes sign between charge and discharge in Eq. (13). At the beginning of the charge, the electrochemical reaction is endothermic and then becomes exothermic over a large part of the charge (see the evolution of $dOCV/dT$ in Fig. 7, which translates the reversible entropic heat by one factor). On discharge, the opposite phenomenon occurs.

5. Conclusion

This paper proposes a 0D thermo-mechanical model of the strain measured with a gauge bonded to the casing surface of a prismatic Li-ion cell. Three contributions have been identified: strain due to Li intercalation, thermal expansion of the casing which is not fully compensated by the second gauge connected to the Wheatstone bridge, and strain due to thermal expansion of the jellyroll. A thermal model has been introduced to describe jellyroll expansion: a steady state model can be used for a low C-rate and a transient model for a high C rate. Experimental tests were carried out to estimate the parameters and characteristics of the thermo-mechanical model: at C/10 rate, the ϵ_{Li} characteristic is extracted as well as the global thermal expansion coefficient α_{cell} defined at low C-rate; at C/5 rate, the reversible entropic heat is estimated as well as the thermal expansion coefficient α_{c-g} related to the casing. The comparison between the model simulation and the measurement performed at 1C rate shows the accuracy of this approach.

However, there is a slight difference with the gauge measurements, which may be due to the mechanical modelling. In this paper, the contribution of the thermal expansion of the jellyroll is assumed to be proportional to the increase in jellyroll thickness ΔL_z calculated without the stress due to the

presence of the casing. Such an assumption is only valid if the materials making up the cell have constant Young's modulus and Poisson's ratio, whatever the strain and the rate of lithiation. By studying the work of Oh [14], it can be argued that this assumption is valid only as a first approximation: their phenomenological approach shows that the cell has a slightly non-linear elastic behaviour and the material properties depend somewhat on the SoC. Future work will address this issue.

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Appendix A. Considerations for modelling mechanical deformation of the casing

For the sake of simplicity, the casing is treated as a thin plate with a thickness e , made of an isotropic material with Young's modulus E_c and Poisson's ratio ν_c ; due to symmetry, only one side of the casing is modelled. Bending the casing results in a displacement $w(x, y)$ along the z -axis defined in the out-of-plane direction, where x and y are the in-plane coordinates (see Fig. 1).

According to the theory of thin plates, $w(x, y)$ is governed by the follow-

ing equation [21]:

$$\frac{\partial^4 w}{\partial x^4} + 2\frac{\partial^4 w}{\partial x^2 \partial y^2} + \frac{\partial^4 w}{\partial y^4} = \frac{q(x, y)}{D_c} \quad (\text{A.1})$$

where q is the normal distributed load on the casing due to the expanding jellyroll and $D_c = \frac{E_c e^3}{12(1-\nu_c^2)}$ the flexural rigidity of the casing.

In the absence of casing, the thickness of the jellyroll would increase by ΔL_z due to thermal expansion, and the displacement $w(x, y)$ would be uniformly equal to $\Delta L_z/2$. The presence of the casing constrains expansion, which limits the displacement $w(x, y)$: jellyroll is therefore compressed. In addition, the jellyroll does not cover the entire surface of the casing: it is free to move in the x- and y-directions. Assuming linear elasticity of the jellyroll, the loading term q in (A.1) can then be written according to Hooke law as follows:

$$q(x, y) = E_j \frac{\Delta L_z/2 - w(x, y)}{L_z/2 + \Delta L_z/2} \quad (\text{A.2})$$

where E_j is the homogenized Young's modulus of the jellyroll [22].

Since $w(x, y) \ll L_z$ and $\Delta L_z \ll L_z$, Eq. (A.2) can be approximated as follows:

$$q(x, y) \approx E_j \frac{\Delta L_z/2 - w(x, y)}{L_z/2} \quad (\text{A.3})$$

By inserting Eq. (A.3) into Eq. (A.1), one obtains:

$$\frac{\partial^4 w}{\partial x^4} + 2\frac{\partial^4 w}{\partial x^2 \partial y^2} + \frac{\partial^4 w}{\partial y^4} + \frac{2E_j}{L_z D_c} w = \frac{E_j}{L_z D_c} \Delta L_z \quad (\text{A.4})$$

Regarding boundary conditions, the difficulty is to model the plate as folded at the edges. Roughly, the edges of the plate can be assumed to be simply supported ($w = 0$ and $\partial^2 w / \partial n^2 = 0$ with n the normal to the edge

defined in xy-plane) or built in ($w = 0$ and $\partial w/\partial n = 0$). In both cases, the boundary conditions do not depend on ΔL_z .

As a consequence, the solution w of Eq. (A.4) with appropriated boundary conditions depends linearly on ΔL_z when linear materials are considered. Furthermore, if the strain ϵ is measured along the x-axis, its expression is given by [21]:

$$\epsilon = \frac{e}{2} \frac{\partial^2 w}{\partial x^2} \quad (\text{A.5})$$

ϵ is also linearly dependent on ΔL_z .

Appendix B. Out-of-plane thermal expansion in the transient case

The solution of Eq. (10) can be formally written as:

$$T(z, t) = \frac{V}{C_{th}} \int_0^t \left(k \frac{\partial^2 T}{\partial z^2} + \frac{\dot{Q}}{V} \right) dt + T_0 \quad (\text{B.1})$$

In the absence of casing, the temperature distribution would generate an out-of-plane thermal expansion, expressed as follows:

$$\Delta L_z(t) = 2 \int_0^{L_z/2} \alpha (T(z, t) - T_0) dz \quad (\text{B.2})$$

Combining Eqs. (B.1) and (B.2), one finds:

$$\begin{aligned} \Delta L_z(t) &= \frac{2\alpha V}{C_{th}} \int_0^{L_z/2} \int_0^t \left(k \frac{\partial^2 T}{\partial z^2} + \frac{\dot{Q}}{V} \right) dt dz \\ &= \frac{2\alpha V}{C_{th}} \int_0^t \int_0^{L_z/2} \left(k \frac{\partial^2 T}{\partial z^2} + \frac{\dot{Q}}{V} \right) dz dt \\ &= \frac{2\alpha V}{C_{th}} \int_0^t \left(\left[k \frac{\partial T}{\partial z} \right]_0^{L_z/2} + \frac{L_z \dot{Q}}{2V} \right) dt \end{aligned} \quad (\text{B.3})$$

Using the boundary conditions given in Eq. (10), one finds:

$$\Delta L_z(t) = \frac{\alpha L_z}{C_{th}} \int_0^t \left(-\frac{2V}{L_z} h(T_s - T_0) + \dot{Q} \right) dt \quad (\text{B.4})$$

which leads to Eq. (11).

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