Structural optimization of electrically charged anodes

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The latest battery developments focus on the design of the anode and try to ensure a safe charging of the electrical device. Here an anode is studied which is made of graphite or silicon and subjected to several physical effects like thermal expansion, electrical current conductivity, and mechanical deformation. Typical design objectives like compliance or conductivity are competing against each other. On the one hand, the compliance is adapted as a design objective and is subjected to a minimization condition by applying external mechanical loads. On the other hand, the conductivity is aimed to be maximized. As a consequence, there is no global optimum structure. Therefore, an univariate optimization of certain objectives is investigated at first. Next, for a bivariate optimization Pareto optimality is used and finite element based numerical simulations are performed. The resulting structures will be used for a simulation of the charging process involving multi-field physics.

1 Introduction

In general, a secondary battery is a multicomponent system composed of anode and cathode material and a separator in between. The design of the anode in rechargeable lithium ion batteries is an ongoing challenge. It addresses the task of maximizing conductivity and mechanical robustness at the same time which requires a multivariate optimization in general.

2 Single objective topology optimization

In the first step we focus on optimization of single objective functions. To this end, we need a domain of interest which is denoted by $\Omega_t \subset \mathbb{R}^3$ in its configuration at time $t$ containing a set of spatial points $x$. The displacement of the reference configuration is given by $u(t) = x(t) - x(0)$. For topology optimization we refer to a finite element discretization of the domain. Within the framework of the SIMP-approach [3] the Young’s modulus $E$ is given for each element $i$ as a convex combination $E_i = E_0(1 - \rho_i^3) + E_1\rho_i^3$ where $E_0$ and $E_1$ are assigned with the limits of the normalized material densities $\rho_i \in [0, 1]$. The global stiffness matrix $K_i = A \left( E_i \int_{\Omega_i} B^T C B \, dV \right)$ results from an assembly operation $A$ over all (sub-) domains $\Omega_i$ based on the strain-displacement matrix $B$ and the constitutive matrix $C$. In the case of conductivity maximization the strategy is similar to the one mentioned above. We interpolate the electrical conductivity $D$ for each element $i$ by $D_i = D_0(1 - \rho_i^4) + D_1\rho_i^4$. This leads to the modified global conductance matrix $K_2 = A \left( D_i \int_{\Omega_i} B^T I B \, dV \right)$ with the identity operator $I$ as a result of the steady-state electric conduction equation. The scalar objective functions are defined by $f_1 = \mathbf{u}^T K_1 \mathbf{u}$ (compliance) and $f_2 = \varphi^T K_2 \varphi$ (conductivity) where $\mathbf{u}$ and $\varphi$ define the global displacement and global voltage vector.

One example of compliance minimization has been already reported in [2] where a cuboid consisting of $40 \times 40 \times 30$ elements is subjected to a single point load on the top side. The emerging optimized structure is a truncated cone and is shown in Figure 1 (c). The same initial geometrical setup has been now chosen to solve a maximum conductivity problem which represents an anode undergoing galvanostatic charging exposed to a constant current. This is implemented as a Neumann boundary condition representing a current directed into the interior of the electrode from below. Furthermore, a zero voltage constraint on top has been applied as Dirichlet boundary condition. The emerging optimized corpus is a hollowed cube, see Fig. 2 (c).

![Fig. 1: (a) Design domain for the minimizing compliance problem. (b) Optimized structure (voxelized plot). (c) Optimized structure (isosurface plot).](image1)

![Fig. 2: (a) Design domain for the maximizing conductivity problem. (b) Optimized structure (voxelized plot). (c) Optimized structure (isosurface plot).](image2)
3 Bi-objective topology optimization

In order to solve a bi-objective topology optimization problem we combine the normalized single objectives $\bar{f}_1$ and $\bar{f}_2$ through a weighted sum $f = w\bar{f}_1 + (1 - w)\bar{f}_2$. The objective functions are normalized by their maximum and so the weighted sum addresses the task of minimizing compliance and maximizing conductivity. The weight factor $w \in [0, 1]$ controls the influence of the objective properties. A full conductive structure results for $w = 0$ and by increasing $w$ the structure becomes less conductive and more stiff until for $w = 1$ we get a fully stiff structure, see Fig. 3. The used optimization code is based on the work of [1].

Fig. 3: Optimized structures (isosurface plot) of the bi-objective topology optimization problem for different weight factors $w$.

4 Chemomechanical coupling

The charging process is based on a coupled chemo-mechanical model which is described in full detail in [4]. Briefly scratched, the mechanical response of the intercalation of the normalized lithium ion concentration $c$ is given by two partial differential equations, e.g. Cahn-Hilliard diffusion $\dot{c} = \nabla \cdot (M\nabla c)$ with mobility $M$, and quasistatic balance of linear momentum $0 = \nabla \cdot \partial \psi / \partial F$ in the framework of finite elasticity. Both equations are linked by the free energy density, which is here

$$\psi = c \ln(c) + (1 - c) \ln(1 - c) + \frac{5}{2} c(1-c) + \kappa |\nabla c|^2 + \sum_i \left[ \frac{K(c)}{4} \left( J_i^2 - 1 - 2 \ln(J_i) \right) + \frac{G(c)}{2} \left( J_i^{-2/3} \text{tr} \left( F^{\top} F \right) - 3 \right) \right]$$

(1)

where $F$ is the deformation gradient and $J = \text{det}(F) = J_e J_i(c)$ its multiplicative decomposed determinant. Both of the elastic moduli $K$ and $G$ are given as a concentration dependent convex combination of the participant species, and $\kappa$ is the gradient energy coefficient. For higher continuity requirement ($C^1$) the volume shown in Fig. 2 (c) is re-meshed by using a spline based formulation, see Fig. 4. For a hollow cube of height 2.5 µm the initial concentration is set to its equilibrium state. A unidirectional ion flux is prescribed from above by a Neumann boundary condition. The structure is fixed at the bottom and embedded at the outer wall sides by a Dirichlet boundary condition, so that it is free to expand only in upward and inward direction. We observe a non-uniform volume swelling and therefore a geometry dependent behavior. In the presented case, the lithium ion concentration accumulates at the corners of the hollow cube, see Fig. 4 (d).

Fig. 4: Sequential color coded concentration evolution shown after (a) 0, (b) 60, (c) 120, (d) 300 time steps.

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