Selection of Container Materials for NaS Batteries towards Higher Thermo-mechanical Stability

Yihan Xu, Chang-Soo Kim*
1Materials Science and Engineering, UWM
*contact at C.-S. Kim (kimcs@uwm.edu) or Y. Xu (yhanxu@uwm.edu)

Introduction to Sodium Sulfur (NaS) Batteries

- Advantages: high energy density, long discharge time, long lifetime, no self-discharge, and low manufacturing costs.
- Applications: grid scale energy storage systems.
- Components: molten electrodes (i.e., Na for anode and S for cathode), δ/β-Al2O3 solid electrolyte (BASE), intricate sealing areas with different types of materials such as metallic alloys or glasses, and outer metallic cell container.

Geometries: planar cells and tubular cells. The advantages of planar NaS cell over tubular cells include the easiness for stacking, inter-cell connection without external connectors, lower manufacturing cost. The active area of the electrode and electrolytes can be sharply defined, and it is also easier to perform post-analysis for cell components. With this, the planar design has been widely used in laboratory conditions.

Objectives

- The thermo-mechanical stress concentrates in the sealing areas during the cell assembly and/or operation processes. Therefore, the thermo-mechanical stability and safety in these joint parts is one of the critical issues in developing commercialized NaS cells, especially for planar cells with increasing cell sizes.
- In this presentation, we introduce the computational finite-element analysis (FEA) approach to address the quantitative assessment of such thermo-mechanical stress concentrations in the joint areas of a planar-type NaS cell with a diameter of 90 mm. Specifically, the impacts of the cell container materials on the thermo-mechanical behavior of the cell will be explored.

Modeling Methods

(1) Procedure
Design cell structure → Construct 3D structure using hyperMesh → Apply BCs, impose static thermal load → ABAQUS solver

(2) Boundary conditions
- 30° slice of a cell, cylindrical coordinate system
- fix the outer edge of bottom surface vertically
- symmetric BCs for both sides of computational cell slice
- tie all the interfaces between adjacent cell components

(3) Material properties

Results and Discussion

Part A. Deformations (shapes) and von-Mises stress distributions (color contours)

Deformations have been multiplied by 10 times for visual purpose, same scale all components.

Part B. Thermo-mechanical stress distribution/accumulation

With the above information, we attempt to analyze the details of the residual stress (i.e., normal stress and shear stress) accumulations on various cell joint areas and BASE.

Conclusions

1. It is suggested to use KOVAR or other alloys to have CTE values smaller than those of STS430 when the planar NaS cell size is large (i.e., greater than 90 mm of BASE disk diameter).
2. It is expected that the current computational model could be readily applied to guide the material selections and to test the thermo-mechanical stability (predict the most likely regions and conditions of potential thermo-mechanical fracture) of contemporary planar NaS cells towards advanced large scale energy storage systems.