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(54) Title: MULTIPHYSICS DESIGN FOR SOLID STATE ENERGY DEVICES WITH HIGH ENERGY DENSITY

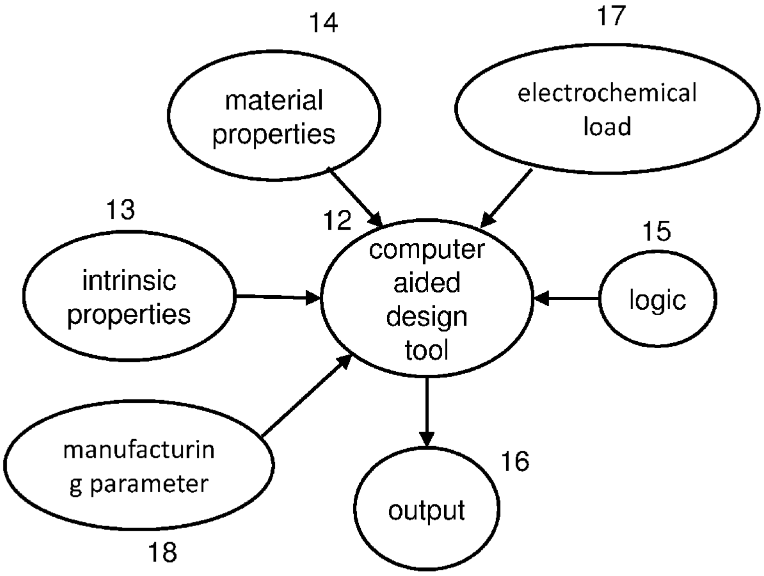

figure 2

(57) Abstract: A method for manufacturing a multi-layered solid state battery. The method includes generating spatial information including an anode geometry, a cathode geometry, a electrolyte geometry, a barrier geometry, and one or more current collector geometries. The method also includes storing the spatial information including the anode geometry, the cathode geometry, the electrolyte geometry, the barrier geometry, and the one or more current collector geometries into a database structure. In a specific embodiment, the method includes selecting one or more material properties from a plurality of materials and using the one or more material properties with the spatial information in a simulation program. The method includes outputting one or more performance parameters from the simulation program.

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MULTIPHYSICS DESIGN FOR SOLID STATE ENERGY DEVICES WITH HIGH ENERGY DENSITY

REFERENCE TO RELATED APPLICATIONS

[0001] This application claims the benefit of U.S. Provisional Application No. 62/094,038, filed December 18, 2014, the content of which is incorporated herein in its entirety by reference.

BACKGROUND OF THE INVENTION

[0002] This present disclosure relates to manufacture of electrochemical cells. More particularly, the present disclosure provides techniques, including a method and device, for a solid state battery device. Merely by way of example, the invention has been provided with use of lithium based battery cells, but it would be recognized that other battery cells made from materials such as zinc, silver and lead, nickel could be operated in the same or like fashion. Additionally, such batteries can be used for a variety of applications such as portable electronics (cell phones, personal digital assistants, radio players, music players, video cameras, and the like), tablet and laptop computers, power supplies for military use (communications, lighting, imaging, satellite, and the like), power supplies for aerospace applications (aero plane , satellites and micro air vehicles), power supplies for vehicle applications (hybrid electric vehicles, plug-in hybrid electric vehicles, fully electric vehicles, electric scooter, , underwater vehicle, boat, ship, electric garden tractor, and electric ride on garden device), power supplies for remote control devices (unmanned aero drone, unmanned aero plane, an RC car), power supplies for a robotic appliances (robotic toys, robotic vacuum cleaner, robotic garden tools, robotic construction utility), power supplies for power tool (electric drill, electric mower, electric vacuum cleaner, electric metal working grinder, electric heat gun, electric press expansion tool, electric saw and cutters, electric sander and polisher, electric shear and nibbler, and routers), power supply for personal hygiene device (electric tooth brush, hand dryer and electric hair dryer), heater, cooler, chiller, fan, humidifier, power supplies for other applications (a global positioning system (GPS) device, a laser rangefinder, a flashlight, an electric street lighting, standby power supply, uninterrupted power supplies, and other portable and stationary electronic devices). The method and system for operation of such batteries are also applicable to cases in which the battery is not the only power supply in the system, and additional power is provided by a fuel cell, other batteries, an IC engine or other combustion devices, capacitors, solar cells, combinations thereof, and others.

[0003] Common electro-chemical cells often use liquid electrolytes. Such cells are typically used in many conventional applications. Alternative techniques for manufacturing electro-chemical cells include solid-state cells. Such solid state cells are generally in the experimental state, have been difficult to make, and have not been successfully produced in large scale. Although promising, solid state cells have not been achieved due to limitations in cell structures and manufacturing techniques. These and other limitations have been described throughout the present specification and more particularly below.

[0004] Conventional manufacturing processes for electrodes involve multiple manufacturing processes. That is, conventional manufacturing of electrodes include casting a paste of mixtures of active materials, conductive additives, binder, and solvent onto a metal substrate to form an electrode. Next, the paste of mixtures making up the electrode is dried in a high temperature oven or at room temperature. The electrode is laminated to a sufficiently low thickness to assure good contact among the constituent particles. Performance targets for electrochemical cells include adequate specific energy/power and energy/power density, cell and module robustness, safety, aging characteristics, lifetime, thermal behavior, and material/shelf life. Unfortunately, limitations exist in designing and manufacturing the electrochemical cells. Achieving the performance targets is accomplished through trial and error, which is tedious and time consuming. Often times, cell capacity and chemistry are selected. The quantity of material for the chemistry is selected for the electrode. The material is provided in one of the three configurations. The resulting battery is tested to determine whether the performance targets have been met, which is generally not the case even after repeated trial and error. Single dimensional simulation within the battery is performed. The amount of active materials used in the electrodes is calculated and recalculated based on targeted capacity. Other parameters including electrode thicknesses, electrolyte compositions, and types and concentrations of additives are typically adjusted until cycle-life and safety targets are met. Clearly, a time- consuming, inefficient, and tedious, process.

[0005] Several published literature reports attempt to provide systematic and numerical approaches to analyzing conventional batteries. These reports pertain to the amount of active materials, conductive additives, binder and porosity of the electrode, and the degree of compression. A pioneering approached was described in "C-W. Wang, and A.M. Sastry, Mesoscale Modeling of a Li-Ion Polymer Cell, Journal of the Electrochemical Society," 154 A1035-A1047 (2007), and Y.-H. Chen, C-W. Wang, G. Liu, X.-Y. Song, V.S. Battaglia, and A.M. Sastry, Selection of Conductive Additives in Li-ion Battery Cathodes: "A Numerical Study, Journal of the Electrochemical Society, 154 A978-A986 (2007)." Although highly successful, such approaches were limited.

[0006] From the above, it is seen that techniques for improving the manufacture of solid state cells are highly desirable. Therefore, to find ways of improving and designing electrochemical cells, which holistically accounts for key manufacturing and performance parameters.

BRIEF SUMMARY OF THE INVENTION

[0007] This present invention relates to manufacture of a multi-layered solid-state battery device. More particularly, the present invention provides a method and system for providing a design and using the design for manufacture of three-dimensional elements for three-dimensional electrochemical cells. Merely by way of example, the invention has been provided with use of lithium based solid state cells, but it would be recognized that other materials such as zinc, silver, magnesium, copper and nickel could be designed in the same or like fashion. Additionally, such batteries can be used for a variety of applications such as portable electronics (cell phones, personal digital assistants, radio players, music players, video cameras, and the like), tablet and laptop computers, power supplies for military use (communications, lighting, imaging, satellite, and the like), power supplies for aerospace applications (aero plane , satellites and micro air vehicles), power supplies for vehicle applications (hybrid electric vehicles, plug-in hybrid electric vehicles, fully electric vehicles, electric scooter, , underwater vehicle, boat, ship, electric garden tractor, and electric ride on garden device), power supplies for remote control devices (unmanned aero drone, unmanned aero plane, an RC car), power supplies for a robotic appliances (robotic toys, robotic vacuum cleaner, robotic garden tools, robotic construction utility), power supplies for power tool (electric drill, electric mower, electric vacuum cleaner, electric metal working grinder, electric heat gun, electric press expansion tool, electric saw and cutters, electric sander and polisher, electric shear and nibbler, and routers), power supply for personal hygiene device (electric tooth brush, hand dryer and electric hair dryer), heater, cooler, chiller, fan, humidifier, power supplies for other applications (a global positioning system (GPS) device, a laser rangefinder, a flashlight, an electric street lighting, standby power supply, uninterrupted power supplies, and other portable and stationary electronic devices). The method and system for operation of such batteries are also applicable to cases in which the battery is not the only power supply in the system, and additional power is provided by a fuel cell, other batteries, an IC engine or other combustion devices, capacitors, solar cells, combinations thereof, and others. The design of such batteries is also applicable to cases in which the battery is not the only power supply in the system, and additional power is provided by a fuel cell, other battery, IC engine or other combustion device, capacitor, solar cell, etc. Merely by way of example, the invention has been provided using finite element analysis or other suitable techniques, a method of numerical analysis of multiphysics problems, in which partial or whole differential equations are solved simultaneously. These relations include, as a partial list, mechanical properties and responses obtained via equilibrium or dynamic load considerations, thermal properties and temperature distributions obtained via heat transfer methods, cell potential and concentrations of species and their transport properties, obtained via kinetic relations and/or fluid flow modeling, among others. Methods including finite difference methods, boundary element analysis, element-free Galerkin (EFG) or Smoothed Particle Hydrodynamics (SPH) methods may also be used. Some, but not all, of these methods employ meshes, or representations of surfaces and volumes, which are generated via a wide range of methodologies, could also be used. Post-processing of data generated in solution of multi-physics problems is described in general, but can be accomplished as a separate step, using any standard method of mining and presenting data.

[0008] In a specific embodiment, an electrochemical cell can be built based on the process of present invention. One or more embodiments of present invention provides a systematic process to manufacturing a three-dimensional electrochemical cell by selecting material characteristics of the three-dimensional electrochemical cells, so that one or more of its performance parameters will meet the design criteria. The material characteristics comprise physical, electrical, thermal, mechanical, optical, or chemical characteristics. The physical characteristics include mass density, crystal structure, stoichiometry, ionic conductivity, diffusivity, and barrier properties including moisture vapor transmission rate (MVTR), water vapor transmission rate (WVTR), and oxygen transmission rate (OTR). The mechanical characteristics include modulus, hardness, thermal expansion coefficient, and concentration expansion coefficient. The electrical characteristics include electronic conductivity, dielectric constant, sheet resistance, and contact resistance. The thermal characteristics include thermal conductivity, specific heat, melting temperature, vaporizing temperature. The optical characteristics include reflectance. The chemical characteristics include reaction constant, open circuit potential. The intrinsic characteristics of the electrochemical cells include layer thickness, layer width, layer length, layer spacing, interfacial interaction of connected layers, shape of each layer, defect size, defect distribution, defect material, type of layer materials. And the selection of electrochemical equilibrium or dynamic load considerations also affect the cell performance parameters. The performance parameters comprises lifetime, safety/physical/mechanical/chemical/thermal/ion concentration, voltage profile, state of charge, degree of intercalation, degree of achievable capacity under various discharge rate or discharge profile, intercalation-induced stresses, or volume changes. In yet an alternative specific embodiment, the present invention provides a method for manufacturing a multi-layered solid-state battery device, the method comprising: generating spatial information each layer geometry. The method also includes storing the spatial information including each layer geometry into a database structure. In a specific embodiment, the method includes selecting one or more material properties from a plurality of materials and using the one or more material properties with the spatial information in a simulation program. In a specific embodiment, the method also includes outputting one or more performance parameters from the simulation program. A multi-layered solid-state battery device comprising a plurality of solid state battery cells numbered from 1 through N, each of the solid state battery cells comprising a first current collector overlying the substrate member, a cathode device overlying the first current collector, an electrolyte device overlying the first current collector, an anode device overlying the electrolyte device, and a second current collector overlying the anode device, each of the plurality of solid state battery cells being operable at a state of charge.

[0009] Still further, the present invention provides a computer-aided system for processing information related to a multi-layered solid-state battery device, the system includes: one or more computer readable memory, the one or more computer readable memory comprising: one or more computer codes for outputting a computer generated relationship between one or more first characteristics referenced against one or more second characteristics for a selected material set for a design of three dimensional spatial elements in a three- dimensional electrochemical cell. One or more codes are directed to selecting one or more of the first characteristics or second characteristics for the selected material set. One or more codes are directed to processing the one or more selected first or second characteristics to determine whether the one or more first or second characteristics is within one or more predetermined performance parameters. One or more codes directed to executing a program for processing the one or more first characteristics or second characteristics to provide the three dimensional electrochemical cell.

[0010] Benefits are achieved over conventional techniques. In one or more embodiments, the present method and system takes an unconventional approach to design an electrochemistry or use of other materials for a selected battery architecture, which is conventionally an ending point and not a starting point for a design process. In a specific embodiment, the present method and system designs an architecture and then determine electrochemistry and other parameters. Accordingly, we have been able to systematically produce a cost effective design and manufacturing process to meet performance targets such as performance, reliability, safety, lifecycle, reclamation and reuse, cost, and other factors. According to the present invention, conventional computer software and hardware can be used for computer aided design of selecting one or more electrochemistries (anode/cathode and electrolyte) for a selected design architecture. In a preferred embodiment, the present method and system can simulate design and processing such as packing in three dimensions, using computer aided hardware and analysis techniques such as mesh generation with irregular geometric objects with memory sizes of 32 gigabyte and greater, and processing speeds of 3 gigahertz and greater. Such irregular shaped objects include, among others, sinusoidal and ellipsoidal. Other benefits include an ability it confers in rational design and combination of multiple materials to produce electrochemical cells, in desired arrangements. These designs, in turn, confer superior properties to designed cells, and elimination of costly-trial and error in construction of prototype cells. Depending upon the specific embodiment, one or more of these benefits may be achieved.

[0011] The present invention achieves these benefits and others in the context of known process technology. However, a further understanding of the nature and advantages of the present invention may be realized by reference to the latter portions of the specification and attached drawings.

BRIEF DESCRIPTION OF THE DRAWINGS

[0012] The following diagrams are merely examples, which should not unduly limit the scope of the claims herein. One of ordinary skill in the art would recognize many other variations, modifications, and alternatives. It is also understood that the examples and embodiments described herein are for illustrative purposes only and that various modifications or changes in light thereof will be suggested to persons skilled in the art and are to be included within the spirit and purview of this process and scope of the appended claims.

[0013] FIGURE 1 is a simplified diagram of a computer aided system for designing a three- dimensional electrochemical cell according to an embodiment of the present invention;

[0014] FIGURE 2 is a simplified diagram of computer modules for the computer aided system for designing the three-dimensional electrochemical cell according to an embodiment of the present invention;

[0015] FIGURE 3 is a simplified diagram of three dimensional processing module according to an embodiment of the present invention;

[0016] FIGURE 4 is a simplified flow diagram of a method for designing an electrochemical cell according to an embodiment of the present invention;

[0017] FIGURE 5A is a simplified flow diagram of the a method for modifying existing electrochemical cell design according to one or more embodiments of the present invention;

[0018] FIGURE 5B is a simplified flow diagram of the a method for modifying existing electrochemical cell manufacturing parameters according to one or more embodiments of the present invention;

[0019] FIGURE 6A illustrates a cathode with thin-film design according to an embodiment of the present invention;

[0020] FIGURE 6B illustrates a cathode with column design according to an embodiment of the present invention;

[0021] FIGURE 6C illustrates a cathode with sinusoidal design according to an embodiment of the present invention;

[0022] FIGURE 7A illustrates an interface of computer aided design process according to an embodiment of the present invention;

[0023] FIGURE 7B illustrates electrochemical cell geometry according to an embodiment of the present invention;

[0024] FIGURE 7C illustrates meshes of an electrochemical cell according to an embodiment of the present invention;

[0025] FIGURE 7D illustrates a contour of lithium concentration at time of 11548 seconds of an electrochemical cell according to an embodiment of the present invention;

[0026] FIGURE 8 is a schematic illustration of multiple stack solid-state batteries by winding according to an example of the present disclosure;

[0027] FIGURE 9 is a schematic illustration of procedure to fabricate multiple stack solid-state batteries by cutting after winding according to an example of the present disclosure;

[0028] FIGURE 10 is a schematic illustration of multiple stack solid-state batteries by z-folding according to an example of the present disclosure;

[0029] FIGURE 11 is a schematic illustration of procedure to fabricate multiple stack solid-state batteries by cutting after z-folding according to an example of the present disclosure;

[0030] FIGURE 12 is a schematic illustration of procedure to fabricate multiple stack solid-state batteries by cutting and stacking according to an example of the present disclosure;

[0031] FIGURE 13 is a schematic illustration of stacked solid state batteries by consecutive deposition processes according to an example of the present disclosure;

[0032] FIGURE 14 is a simplified illustration of contour plot showing the discharge volumetric energy density (in Wh/l) of a cell design when discharged at C/10 with different low and high cut-off voltages according to an example of the present disclosure.

[0033] FIGURE 15 is a simplified illustration of contour plot showing the operational time (in min) of a cell designed for high power applications with different low and high cut-off voltages according to an example of the present disclosure.

[0034] FIGURE 16 is a simplified illustration of contour plot showing the operational time (in min) of a cell, with improved material properties by adjusting processing conditions, designed for high power applications with different low and high cut-off voltages according to an example of the present disclosure.

[0035] FIGURE 17 is a simplified illustration of contour plot showing the discharge volumetric energy density (in Wh/l) of a cell designed for wearable device applications with different low and high cut-off voltages according to an example of the present disclosure.

[0036] FIGURE 18 is a simplified illustration of contour plot showing the discharge volumetric energy density (in Wh/l) of a cell, with improved material properties by adjusting processing conditions, designed for wearable device applications with different low and high cut-off voltages according to an example of the present disclosure.

[0037] FIGURE 19 is an illustration of cathode diffusivity as a function of normalized distance by cathode thickness from cathode current collector (CC) and cathode (CA) interface.

[0038] FIGURE 20 is an illustration of the simulation result of lithium trapped in cathode over cycle.

[0039] FIGURE 21 is a schematically representation of function graded materials according to an example of the present disclosure.

[0040] FIGURE 22A is a representation of diffusivity as a function of CC/CA interface distance in functionally graded materials according to an example of the present disclosure.

[0041] FIGURE 22B shows the lithium ion concentration profile in the cathode at different discharge rate.

[0042] FIGURE 23 is an illustration of effect electrolyte electronic conductivity on open circuit potential over time.

[0043] FIGURE 24 is a schematic representation of fabrication a multiple stacked solid state battery cells on an arbitrary shape of mandrel as winding during deposition according to an example of the present disclosure.

[0044] FIGURE 25 is a schematic representation of winding multiple stacked solid state battery cells on an arbitrary shape of mandrel from a deposited drum according to an example of the present disclosure.

[0045] FIGURE 26A is a schematic representation of multiple stacked solid state battery integrated into the ring shape frame of a portable fan.

[0046] FIGURE 26B is a list of simplified illustrations of arbitrary configuration of a multiple stacked solid state battery cells according to an example of the present disclosure.

DETAILED DESCRIPTION OF THE INVENTION

[0047] According to the present invention, techniques related to manufacture of electrochemical cells are provided. More particularly, the present invention provides a method and system for providing a design and using the design for manufacture of three-dimensional elements for three-dimensional electrochemical cells. Merely by way of example, the invention has been provided with use of lithium based cells, but it would be recognized that other materials such as zinc, silver, magnesium, copper and nickel could be designed in the same or like fashion.

[0048] Additionally, such batteries can be used for a variety of applications such as portable electronics (cell phones, personal digital assistants, radio players, music players, video cameras, and the like), tablet and laptop computers, power supplies for military use (communications, lighting, imaging, satellite, and the like), power supplies for aerospace applications (aero plane , satellites and micro air vehicles), power supplies for vehicle applications (hybrid electric vehicles, plug-in hybrid electric vehicles, fully electric vehicles, electric scooter, , underwater vehicle, boat, ship, electric garden tractor, and electric ride on garden device), power supplies for remote control devices (unmanned aero drone, unmanned aero plane, an RC car), power supplies for a robotic appliances (robotic toys, robotic vacuum cleaner, robotic garden tools, robotic construction utility), power supplies for power tool (electric drill, electric mower, electric vacuum cleaner, electric metal working grinder, electric heat gun, electric press expansion tool, electric saw and cutters, electric sander and polisher, electric shear and nibbler, and routers), power supply for personal hygiene device (electric tooth brush, hand dryer and electric hair dryer), heater, cooler, chiller, fan, humidifier, power supplies for other applications (a global positioning system (GPS) device, a laser rangefinder, a flashlight, an electric street lighting, standby power supply, uninterrupted power supplies, and other portable and stationary electronic devices). The method and system for operation of such batteries are also applicable to cases in which the battery is not the only power supply in the system, and additional power is provided by a fuel cell, other batteries, an IC engine or other combustion devices, capacitors, solar cells, combinations thereof, and others.

[0049] Merely by way of example, the invention has been provided using a method of numerical analysis of multiphysics problems, in which partial or whole differential equations are solved simultaneously. These relations include material characteristics, intrinsic characteristics, electrochemical equilibrium or dynamic load considerations, and performance parameters. The material characteristics comprise physical, electrical, thermal, mechanical, optical, or chemical characteristics. The physical characteristics include mass density, crystal structure, stoichiometry, ionic conductivity, diffusivity, and barrier properties including moisture vapor transmission rate (MVTR), water vapor transmission rate (WVTR), and oxygen transmission rate (OTR). The mechanical characteristics include modulus, hardness, thermal expansion coefficient, and concentration expansion coefficient. The electrical characteristics include electronic conductivity, dielectric constant, sheet resistance, and contact resistance. The thermal characteristics include thermal conductivity, specific heat, melting temperature, vaporizing temperature. The optical characteristics include reflectance. The chemical characteristics include reaction constant, open circuit potential. The intrinsic characteristics of the electrochemical cells include layer thickness, layer width, layer length, layer spacing, interfacial interaction of connected layers, shape of each layer, defect size, defect distribution, defect material, type of layer materials. The shape of each layer comprises flat, periodic patterned, or irregular shape, or combinations of these, and shape of each layer is independent of other layers. And the layer of three dimensional electrochemical cell is selected from homogenous materials, inhomogenous materials or graded materials, or any combination of these. And the graded materials comprise variation in composition and material structure over the volume of the layer. And material structure comprise crystalline structure, or amorphous structure, or any combination of these. The performance parameters comprises lifetime, safety/physical/mechanical/chemical/thermal/ion concentration, voltage profile, state of charge, degree of intercalation, degree of achievable capacity under various discharge rate or discharge profile, intercalation-induced stresses, or volume changes. The numerical method is selected from a finite element method, a finite element method (FEM), a finite difference method (FDM), a boundary element analysis, element-free Galerkin (EFG) or Smoothed Particle Hydrodynamics (SPH) method and the numerical method employs meshes or representations of surfaces and volumes. Some, but not all, of these methods employ meshes, or representations of surfaces and volumes, which are generated via a wide range of methodologies, could also be used. Post-processing of data generated in solution of multiphysics problems is described in general, but can be accomplished as a separate step, using any standard method of mining and presenting data. The design of such batteries is also applicable to cases in which the battery is not the only power supply in the system, and additional power is provided by a fuel cell, other battery, IC engine or other combustion device, capacitor, solar cell, etc.

[0050] FIGURE 1 illustrates a computer system for computer-aided design for an electrochemical cell, wherein a computer 1, responds to inputs from keyboard 2, and/or other digitizing input device such as a light pen, or a mouse 3, and displays designs of the three-dimensional electrochemical cell on the graphical display device 4. This diagram is merely an illustration and should not unduly limit the scope of the claims herein. One of ordinary skill in the art would recognize many variations, modifications, and alternatives.

[0051] Commercially available, or in-house developed simulation programs and database are stored in the electronic storage device 5, which may be a magnetic disk or other type of digitized data storage device. As described throughout the present specification, a database is provided and used to gather electrochemical cell information and couple the electrochemical cell information to a three-dimensional simulation program. In a computer graphics aided design, morphologic information is displayed on the graphical display device 4. As a simple example, the three-dimensional electrochemical cell is shown, wherein anode, cathode, electrolyte, and two current collectors are shown. Typically, a simulation program is loaded from the storage device 5, through the bridge unit 6, into the memory unit 7, as a whole. Then, the digitized rendering of the three-dimensional electrochemical cell is loaded either from the data storage device 5, or input devices 2 and 3. Data include geometric information and material properties. In a specific embodiment, the method obtains a battery and reverse engineers it to determine the information, such as materials, configuration, geometry, and any and all other measurable parameters. Alternatively, the present method selects one or more materials and determines their properties, including extrinsic and intrinsic, according to a specific embodiment. Multiple programs are added to the base structure from the mass storage device 5 and then processed using device 8. These added programs include a meshing algorithm, a solver algorithm, a postprocessing algorithm, and the like. The post-processed data then are sent back to the database structure, resulting in changes in database. Finally, the whole data structure and simulation programs are streamlined, and stored in the data storage device 5. The database stored in the data storage device 5 includes material characteristics, intrinsic characteristics, electrochemical equilibrium or dynamic load considerations, and performance parameters. The manufacturing parameters for thin film deposition is also stored in the storage so one can build the relationships among manufacturing parameters and material characteristics, intrinsic characteristics, electrochemical equilibrium or dynamic load considerations, and performance parameters.

[0052] FIGURE 2 depicts the tool 12 of the present invention regarding computer-aided design of a three-dimensional electrochemical cell, wherein all of the programs for generating the geometric layout, the logic, and solving required equations are integrated. This diagram is merely an illustration and should not unduly limit the scope of the claims herein. One of ordinary skill in the art would recognize many variations, modifications, and alternatives. The intrinsic 13 includes layer thickness, layer width, layer length, layer spacing, interfacial interaction of connected layers, shape of each layer, defect size, defect distribution, defect material, type of layer materials. The material properties 14 include physical, electrical, thermal, mechanical, optical, or chemical characteristics and they are input as part of the database structure. The material properties, M(x_i,y_i,z_i) are included in the database structure. M is the material property index and i is the layer index. The material properties include homogenous materials, inhomogenous materials or graded materials, or any combination of these. And the graded materials comprise variation in composition and material structure over the volume of the layer. In an example functionally graded properties can also include electrical conductivity σ(x,y,z), dielectric constant ε(x,y,z), mass density ρ(x,y,z), modulus E(x,y,z), thermal conductivity κ(x,y,z), thermal expansion coefficient α(x,y,z), thermal specific heat □□(x,y,z), concentration expansion α□(x,y,z), reaction constant κ0(x,y,z), and electropotential E(x,y,z). The logic 15, underlies the behavior of the materials. The electrochemical load 17, underlies electrochemical equilibrium or dynamic load considerations including cell charge, discharge current, voltage, and time profile. The manufacturing parameters 18, underlies the manufacturing process parameters to make multi-layered solid state battery device. Then, the operation of the three-dimensional electrochemical cell is simulated based on the information gathered by this computer aided design tool, and is output to the database structure 16.

[0053] FIGURE 3 illustrates the simulation program 25 used as an engine of the present invention. This diagram is merely an illustration and should not unduly limit the scope of the claims herein. One of ordinary skill in the art would recognize many variations, modifications, and alternatives. The program integrates the input data, the logic, meshing algorithm, solving algorithm, and the post-process algorithm together. This simulation program could be obtained commercially or built in-house. The input data includes the geometric information 26 and the material properties 19. The governing equations 20 and boundary equations 21 are chosen based on the underlying logic for the material behaviors. The meshing algorithm 22 chooses the order of the governing and boundary equations and provides the degree of the approximation to the real material behaviors. The solver algorithm 23 provides the efficiency and accuracy of the end results. The post-process algorithm 24 provides showing the computational results, and showing results in terms graphics', charts', or tables' forms. The electrochemical load 27, underlies electrochemical equilibrium or dynamic load considerations including cell charge, discharge current, voltage, and time profile. In a specific application of the present invention, a systematic process for manufacturing a new electrochemical cell is made possible, as depicted in FIGURE 4.

[0054] (1) The designer generates necessary geometric information of a multi-layered solid state battery. In the present invention, the electrode morphology is not limited into thin-film shape, but also includes any three-dimensional geometries or combination of three-dimensional geometries including flat, patterned, or irregular shapes. The designer also selects electrochemical load.

[0055] (2) The database is then loaded into the finite element method simulation program.

[0056] (3) The designer inputs the material properties into the database structure.

[0057] (4) The designer selects the proper governing equations and boundary equations to interpret the behavior of the involving materials, such as the anode, cathode, electrolyte, electrolyte, barrier, and current collectors.

[0058] (5) The finite element method simulation program gathers the structural database regarding the geometric and material information, governing and boundary equations, and solver algorithm to obtain the operational performance parameters.

[0059] (6) The designer then compares the simulation results and the desired performance parameters. If the errors between simulated results and desired performance parameters are within acceptable tolerances, the simulated setup of the three-dimensional electrochemical cell is accepted. If the errors are not within the acceptable tolerances, the design of the three- dimensional electrochemical cell is systematically changed and the design process (1) to (6) is repeated until errors are within the acceptable tolerance.

[0060] In another application with present invention, an existing electrochemical cell design is modified, as depicted in FIGURE 5A.

[0061] 1) The designer generates the geometric and material properties information for the multi-layered solid state battery for entry into the database structure for the existing electrochemical cell design.

[0062] 2) The database is then loaded into the computer aided design tool depicted in FIGURE 2 to simulate the electrochemical cell performance for the existing design.

[0063] 3) In parallel, the designer generates the geometric, material properties, electrochemical load information as the database structure for the modified electrochemical cell design.

[0064] 4) The database is then loaded into the computer aided design tool depicted in FIGURE 2, to simulate the electrochemical cell performance for the modified design.

[0065] 5) Then, the designer compares the two cell performances obtained from process 2) and 4) to determine whether the modified design is acceptable.

[0066] 6) If the performance of the modified design is acceptable, the final product is built based on the modified design.

[0067] 7) If the performance of the modified design is unacceptable, the designer systematically repeats processes 3) to 7) until the cell performance is acceptable.

[0068] In another application with present invention, an existing electrochemical cell design is modified, as depicted in FIGURE 5B.

[0069] 1) The designer generates the geometric and material properties information for the multi-layered solid state battery for entry into the database structure for the existing electrochemical cell design.

[0070] 2) The database is then loaded into the computer aided design tool depicted in FIGURE 2 to simulate the electrochemical cell performance for the existing design.

[0071] 3) In parallel, the designer generates the geometric, material properties, electrochemical load information as the database structure for the modified electrochemical cell design.

[0072] 4) The database is then loaded into the computer aided design tool depicted in FIGURE 2, to simulate the electrochemical cell performance for the modified manufacturing parameters.

[0073] 5) Then, the designer compares the two cell performances obtained from process 2) and 4) to determine whether the modified manufacturing parameters are acceptable.

[0074] 6) If the performance of the modified manufacturing parameters are acceptable, the final product is built based on the modified design.

[0075] 7) If the performance of the modified design is unacceptable, the designer systematically repeats processes 3) to 7) until the cell performance is acceptable.

EXAMPLE 1 Design and Method of an Electrochemical Cell

[0076] This example demonstrates the process of manufacturing a new electrochemical cell with the optimal morphological shape of the electrode. As an example, multi-layered solid-state battery with stack number 1 is designed and manufactured. As an example of the problems encountered by the designer, three different morphological designs of three-dimensional electrodes are provided: thin-film in FIGURE 6A, columnar shape in FIGURE 6B, and a sinusoidal shape in FIGURE 6C. The materials for the three-dimensional electrochemical cells are copper as anode current collector (33 in FIGURE 6A, 38 in FIGURE 6B, 43 in FIGURE 6C), lithium metal as anode (34 in FIGURE 6A, 40 in FIGURE 6B, 45 in FIGURE 6C), lithium manganese oxide as cathode (36 in FIGURE 6A, 41 in FIGURE 6B, 46 in FIGURE 6C), polymer with lithium salts as the electrolyte (35 in FIGURE 6A, 39 in FIGURE 6B, 44 in FIGURE 6C), and aluminum as cathode current collector (37 in FIGURE 6A, 42 in FIGURE 6B, 47 in FIGURE 6C). The material properties, M(x_i,y_i,z_i) are selected from the database structure. M is the material property index and i is the layer index. The material properties include homogenous materials, inhomogenous materials or graded materials, or any combination of these. And the graded materials comprise variation in composition and material structure over the volume of the layer. In an example functionally graded properties can also include electrical conductivity $\sigma(x,y,z)$, dielectric constant $\varepsilon(x,y,z)$, mass density $\rho(x,y,z)$, modulus E(x,y,z), thermal conductivity $\kappa(x,y,z)$, thermal expansion coefficient $\alpha(x,y,z)$, thermal specific heat □□(x,y,z), concentration expansion α□(x,y,z), reaction constant $\kappa 0(x,y,z)$, and electropotential E(x,y,z). These materials used here are for illustrative purposes, but are not limited by these materials. The volume of the three different design electrodes are constraints. Designers using conventional systems would often go into the laboratory and build these three different designs of cathode, assemble them into real cells, and test them for a period of time to obtain the performance parameters. Designer can obtain the performance parameters by using one or more embodiments of the present invention more efficiently.

[0077] Then, present computer- aided design process (as 60-70 in FIGURE 8A), which has been integrated as (71) in FIGURE 8A, will simulate the database structure and output the outcome of the two designs. The designer will collect the particle size and volume fraction based on the image analysis techniques or from the original design database to generate the geometry of the cell as (72) in FIGURE 8B by clicking on "CAD" button (60 in FIGURE 8A). Then, the designer inputs the material properties by clicking on "Material Properties" button (61 in FIGURE 8A), and the inputs the governing equations and boundary conditions for intended cell behaviors by clicking on "Governing Equations" and "Boundary Conditions" buttons (62 and 63 in FIGURE 8A), respectively. Then, the meshes will be generated as shown (84 in FIGURE 8C) by clicking on "Meshing" button. Next, the designer will chose the solver to solve the results by clicking on "Solver" button (as 90 in FIGURE 8C). Final results can be presented in terms of the table or contours as shown 96 in FIGURE 8D by clicking on 91 in FIGURE 8C. The designer then compares the two performance parameters. If the outcome of the new design is satisfied with the target performance characteristic, the final electrochemical cell will be manufactured by the newer design. If it is not satisfied, the designer could modify the new design with new idea repeatedly with the same process until the performance parameters is satisfied. Again, any of the diagrams herein are merely illustrations and should not unduly limit the scope of the claims herein. One of ordinary skill in the art would recognize many variations, modifications, and alternatives.

[0078] This example result demonstrates it could identify two important factors that will affect the rate performance, durability, and life of the electrochemical cell. The first factor is the sharp corner of the column shape of electrode. As in this example, the maximum intercalation induced stress of column shape design is about four times larger than the thin-film design. The other factor is the surface-to-volume ratio of the cathode. It is believed that sharp corner will intensify the stress, which will result in short life and low durability. On the other hand, the small surface- to-volume ratio will result in low charge/discharge rate capability. As in this example, the maximum achievable capacity under 1C rate, which regulates the discharge current so that ideally the whole capacity of the cell will be exhausted within one hour, for the thin-film design is about 73% of the column shape design. Hence, the sinusoidal design is the optimal design in this case.

EXAMPLE 2 Building multiple stack solid state batteries by winding

[0079] This example demonstrates building multiple stack solid state batteries by winding. As an example, the present invention provides a method of using a flexible material that has a thickness in the range between 0.1 and 100 μm as the substrate for the solid state batteries. The flexible material can be selected from polymer film, such as PET, PEN, or metal foils, such as copper, aluminum. The deposited layers that comprise solid state batteries on the flexible substrate, then can be wound into a cylindrical shape or wound then compressed into a prismatic shape. FIGURE 8 shows the image of the wound cell as an example of the present invention. The wound cells can further be processed by cutting the round corners to maximize the energy densities as shown in FIGURE 9.

EXAMPLE 3 Building multiple stack solid state batteries by z-folding

[0080] This example demonstrates building multiple stack solid state batteries by z-folding. As an example, the present invention provides a method of using a flexible substrate that can be a part of solid state batteries. As shown in FIGURE 10, the deposited layers of solid state batteries on the flexible substrate can be stacked by z-folding. The z-folded cells can further be processed by cutting two sides of cells and terminating them to maximize the energy densities as shown in FIGURE 11. By alternating the process sequence, another configuration of multistack battery can be made by cutting the individual layers and then stacking them as illustrated in FIGURE 12.

EXAMPLE 4 Building multiple stack solid state batteries by iterative deposition process

[0081] This example demonstrates building multiple stack solid state batteries by iterative deposition process: As an example, the present invention provides a method of building multiple stack solid state batteries by moving a substrate through a number of deposition processes. By repeating a sequence of processes by N times, the solid state battery device has N number of stacks as shown in the schematic diagram in FIGURE 13.

EXAMPLE 5 Designed energy density by controlling SOC, contour plot

[0082] Because solid state batteries have much higher energy densities than conventional batteries, these batteries are capable of delivering very high energy density even cycled at limited state of charge, SOC (not full SOC range). In the example, multiphysics finite element simulation is used for designing energy density by controlling SOC. FIGURE 14 shows the discharge volumetric energy density (in Wh/l) of an example cell design when discharged at C/10 at different high and low cut-off voltages. It is shown that there are very wide range of options which can deliver energy densities greater than 700 Wh/l (or 800 Wh/l or 900 Wh/l or 1000 Wh/l).

EXAMPLE 6 Designed operational time for high power applications by controlling SOC, for high power

[0083] Because solid state batteries have much higher energy densities than conventional batteries, these batteries are capable of delivering very high energy density even cycled at limited SOC (not full SOC range). In the example, multiphysics finite element simulation is used for designing operational time for high power applications. For a specific high power application using such batteries, the application device can operate longer time using such batteries. FIGURE 15 shows the operational time (in minutes) of an example cell design when discharged at a very high power of 25 W at different high and low cut-off voltages.

[0084] Battery material properties can also be adjusted by tuning processing parameters, such as background gas types, background gas partial pressure, and substrate temperature. As an example, increasing gas pressure will result in decrease in mass density and increase in diffusivity. As another example, by changing the gas type, we can change the concentration of different species in the film composition. After battery material properties are adjusted by tuning processing parameters, the battery can meet the target energy density application. FIGURE 16 shows the operational time (in minutes) of an example cell design with improved material properties when discharged at a very high power of 25 W at different high and low cut-off voltages. In this cell design, cells are deposited on a thin flexible substrate.

EXAMPLE 7 Designed energy density for cells targeting wearable device applications

[0085] Because solid state batteries have much higher energy densities than conventional batteries, these batteries are capable of delivering very high energy density even cycled at limited SOC (not full SOC range). In the example, multiphysics finite element simulation is used for designing energy density for cells targeting wearable device applications. For a specific wearable device application using such batteries, FIGURE 17 shows the deliverable energy density of an example cell design when discharged at 67 mA at different high and low cut-off voltages.

[0086] Battery material properties can also be adjusted by tuning processing parameters to meet the target energy density application. FIGURE 18 shows the deliverable energy density of an example cell design with improved material properties when discharged at 67 mA at different high and low cut-off voltages. In this cell design, cells are deposited on a thin flexible substrate.

EXAMPLE 8 Capacity fade and lithium trapped in cathode due to graded cathode diffusivity

[0087] In the example, functionally graded cathode material is made where the top part has very high lithium ion diffusivity and the bottom part has very low diffusivity. In the example, multiphysics finite element simulation is used for trapped lithium calculation in cathode. FIGURE 19 shows the cathode diffusivity as a function of normalized distance by cathode thickness from cathode current collector (CC) and cathode (CA) interface. Functionally graded material with very low lithium diffusivity near current collector side and very high lithium diffusivity in the other side is made. The cell is discharged at 1C rate, and constant current charged at 1C rate, followed by constant voltage charge with 2 hours of holding time. Due to the variation of diffusivity in cathode, not all the lithium can transport in time during cycling. FIGURE 20 shows the result of lithium trapped in cathode over cycle. After 16 cycles, 2% of lithium (2% of capacity) is trapped in the cathode.

EXAMPLE 9 Functionally graded cathode material and capacity retention

[0088] In an example, the present disclosure describes the unexpected benefits of controlling state of charge in solid state battery cathodes with functionally graded properties. Functionally graded materials (FGM) can be characterized by the variation in composition and structure gradually over volume, resulting in corresponding changes in the properties of the material. As an example in FIGURE 21, a cathode is made such that mass density decreases as deposition progresses by controlling the process pressure during deposition. In such a battery, less dense material on the top of cathode close to an electrolyte has higher lithium ion diffusivity, thus works better for high power application. Lower diffusivity at a region close to current collectors prevents lithium diffusion through the cathode down to the current collectors. This functionally graded cathode material containing high diffusivity region near the electrolyte and low diffusivity region at the bottom adjacent to the current collector provides unique combination for both high power performance and capacity retention. In an example, the lower diffusivity region has a diffusivity ranging from 1×10^{-19} m2/s to 1×10^{-5} m2/s and the higher diffusivity has a diffusivity value ranging from 1×10^{-17} m2/s to 1×10^{-5} m2/s. In an example functionally graded properties can also include electrical conductivity $\sigma(x,y,z)$, dielectric constant $\varepsilon(x,y,z)$, mass density $\rho(x,y,z)$, modulus $E(x,y,z)$, thermal conductivity $\kappa(x,y,z)$, thermal expansion coefficient $\alpha(x,y,z)$, thermal specific heat □□(x,y,z), concentration expansion α□(x,y,z), reaction constant $\kappa 0(x,y,z)$, and electropotential $E(x,y,z)$. In an example, FGM cathode diffusivity only varies in one dimension (z-direction) and is constant in x- and y-directions. In another example, cathode diffusivity varies in the x-z, y-z, and x-y planes. The present disclosure provides a method of utilizing these advantages of cathode and solid state batteries by defining and controlling the voltage range and the depth of discharge.

[0089] In an example, cathode material with functionally graded diffusivity and constant diffusivity are made. The functionally graded cathode with linear diffusivity distribution of cathode where the top part has higher lithium ion diffusivity and the bottom part has lower diffusivity, and the diffusivity distribution is shown in FIGURE 22A. In the example, multiphysics finite element simulation is used for lithium concentration calculation in cathode. FIGURE 22B shows the lithium ion concentration profile in the cathode at different discharge rate and in different cathode material. If the target is high utilization of lithium, C/10 is recommended in the application for both graded diffusivity and constant diffusivity cathode materials. If the low lithium ion concentration at the CC/CA interface is required in order to prevent lithium diffusion through CC, 1C discharge rate and graded cathode material are recommended in the application.

EXAMPLE 10 Self-discharge and current leakage in electrolyte due to defect. In an example, the present disclosure describes the effect of defect in the electrolyte layer using finite element multi-physics simulation. Pinhole, crack, spit, and debris are common defects in electrolyte made by deposition technique. With increase the defect size and distribution in the electrolyte, the electronic conductivity increases, which result in drop in open circuit potential. FIGURE 23 shows the effect of electrolyte electronic conductivity on open circuit potential over time. With increase in the electronic conductivity, the cell self-discharges and the voltage drops over time.

Defects need to be reduced in order to keep the low electronic conductivity in the electrolyte to maintain low self-discharge rate and long battery life.

EXAMPLE 11 winding solid state battery cells on arbitrary shape of mandrel, FIGURE 17 shows schematically the winding solid state battery cells on mandrel **1701**, and deposition means. This is as an example of deposition of multiple stack solid state battery cells with arbitrary shape of mandrel, but it is not limited to the shape illustrated here. In this example, the cross section of 8-shape can be as vacuum cleaner handle part. The vacuum cleaner handle part can be used as the substrate for solid state battery cells. In one of the specific embodiment of current invention, the multiple stacked solid state battery cells can be achieved by depositing each cell components sequentially, from first current collector, cathode, electrolyte, anode, second current collector, and insulating interlayer. This deposition sequence will be repeated 1 to N times until desired total capacity achieved. Because of the thin layer characteristics, the increased volume of the stick vacuum would be minimumized compared to conventional liquid or polymer gel types of battery cells. In this example, there are needs to have push rollers as **1704, 1705** and **1706** to assist the deposition battery cells **1703** conformably stick on the mandrel. As the mandrel rotating, the push rollers would need to move along the surface so that they would not be on the way of the rotation. Furthermore, the deposition sources are located under the mandrel as an example. However, the location of the deposition source can be located in any location around the mandrel to achieve uniformity of the multiple stacked solid state battery cells. The required deposition sources will be moved into the positions when they are needed. The deposition sources can also be positioned based the shape of the mandrel. For example, the two different layer deposition sources can be position on the opposite side of the 8 shape mandrel due to wide shade shielding characteristics to minimize the deposition time.

EXAMPLE 12 winding on arbitrary shape of mandrel, FIGURE 18 shows schematically the winding on mandrel **1803**. This is as an example of deposition of multiple stack solid state battery cells with arbitrary shape of mandrel, but it is not limited to shape illustrate here. In this example, the cross section of 8 shape can be as a vacuum cleaner handle part. In one of the specific embodiment of current invention, the multiple stack solid state battery cells can be achieved by depositing each cell components sequentially on another drum or mandrel **1801**, from first current collector, cathode, electrolyte, anode, second current collector, and insulating interlayer. This deposition sequence will be repeated 1 to N time until desired total capacity achieved. Once the desired total capacity achieved, rolled solid state battery cells will be move to winding station. On the winding station, the desired shape mandrel will be used to load the solid state battery cell. The deposited solid state battery cells will be unloaded from the cylindrical drum and winded to the desired shape mandrel, as in this example, 8-shape mandrel. After wounded to the 8-shape mandrel, the final packaging layer will be layered on top of the battery to provide insulation to environment. Because of the thin layer characteristics, the increased volume of the vacuum cleaner handel would be minimum compared to conventional liquid or polymer gel types of battery cells. In this example, there are needs to have push rollers as **1804, 1805** and **1806** to assist the winding battery cells **1802** conformably stick on the mandrel surface. As the mandrel rotating, the push rollers would need to move along the surface so that they would not be on the way of the rotation.

EXAMPLE 13 Integrating the multiple stack solid state batteries to the structural and/or decorative space of application device: As an example, the present invention provides a method of forming solid state batteries into a shape as in FIGURE 26A. The solid state batteries on a flexible substrate disclosed in this present invention can form any arbitrary shape. A multiple stack battery device **2205** is wound on a hollow core to be used within a housing **2202** of a bladeless fan or an air blower **2201** as shown in FIGURE 26A. Multiple stack battery **2205** integrated to the structure, for example the rim of the fan head **2204**, eliminates the need of having a separate space for storage, allowing design only needed for the function of the appliance while enabling portability. FIGURE 26B demonstrates some of the example form factors that the flexible batteries may have, such as a torus, a coil, a circular cone, a trapezoidal cone, and a tetrahedron.

CLAIMS

1. A method for designing a multi-layered solid-state battery device: providing computer generated relationship between one or more first characteristics referenced against one or more second characteristics for a selected material set for design of three dimensional spatial elements in a three-dimensional electrochemical cell; selecting one or more of the first or second characteristics for the selected material set; processing the one or more selected first or second characteristics to determine whether the one or more first or second characteristics is within one or more predetermined performance parameters; and using the one or more first or second characteristics to design of the three dimensional multi-layered solid-state battery device.

2. The method of claim 1 wherein a multi-layered solid-state battery device comprising a plurality of solid state battery cells numbered from 1 through N, each of the solid state battery cells comprising a first current collector overlying the substrate member, a cathode device overlying the current collector, an electrolyte device overlying the cathode, an anode device overlying the electrolyte device, and a second current collector overlying the anode device, each of the plurality of solid state battery cells being operable at a state of charge.

3. The device of claim 1 wherein the plurality of battery cells is wound or stacked.

4. The method of claim 1 wherein the one or more first characteristics comprise physical, electrical, thermal, mechanical, optical, or chemical characteristics.

5. The method of claim 4 wherein physical characteristics comprise but not limited to mass density, crystal structure, stoichiometry, ionic conductivity, diffusivity, moisture vapor transmission rate (MVTR), water vapor transmission rate (WVTR), and oxygen transmission rate (OTR).

6. The method of claim 4 wherein mechanical characteristics comprise but not limited to modulus, hardness, thermal expansion coefficient, and concentration expansion coefficient.

7. The method of claim 4 wherein electrical characteristics comprise but not limited to electronic conductivity, dielectric constant, sheet resistance, and contact resistance.

8. The method of claim 4 wherein thermal characteristics comprise but not limited to thermal conductivity, specific heat, melting temperature, vaporizing temperature.

9. The method of claim 4 wherein optical characteristics comprise but not limited to reflectance.

10. The method of claim 4 wherein chemical characteristics comprise but not limited to reaction constant, open circuit potential.

11. The method of claim 1 wherein the one or more second characteristics comprise layer thickness, layer width, layer length, layer spacing, interfacial interaction of connected layers, shape of each layer, defect size, defect distribution, defect material, type of layer materials, or electrochemical equilibrium or dynamic load considerations.

12. The method of claim 1 wherein the shape of each layer comprises flat, periodic patterned, or irregular shape, or combinations of these, and shape of each layer is independent of other layers.

13. The method of claim 1 wherein the performance parameters comprises lifetime, safety/physical/mechanical/chemical/thermal/ion concentration, voltage profile, state of charge, degree of intercalation, degree of achievable capacity under various discharge rate or discharge profile, intercalation-induced stresses, or volume changes.

14. The method of claim 1 wherein the layer of three dimensional electrochemical cell is selected from homogenous materials, inhomogenous materials, or graded materials, or any combination of these.

15. The method of claim 14 wherein the graded materials comprise variation in composition and material structure over the volume of the layer.

16. The method of claim 15 wherein material structure comprise crystalline structure, or amorphous structure, or any combination of these.

17. A method for analyzing a three-dimensional multi-layered solid-state battery device, the method comprising: using a numerical method to process one or more relationships, the one or more relationships being one or more coupled or decoupled, continuous, discretized, or piecewise continuous, partial or whole differential equations or other logical forms; determining one or more first or second characteristics in a first three-dimensional electrochemical cell; generating a relationship between the one or more first characteristics referenced against the one or more of the second characteristics; processing the one or more selected first or second characteristics to determine whether the one or more first or second characteristics is within predetermined performance parameters; and using the one or more first or second characteristics for a second three dimensional electrochemical device.

18. The method of claim 17 wherein a multi-layered solid-state battery device comprising a plurality of solid state battery cells numbered from 1 through N, each of the solid state battery cells comprising a first current collector overlying the substrate member, a cathode device overlying the first current collector, an electrolyte device overlying the first current collector, an anode device overlying the electrolyte device, and a second current collector overlying the anode device, each of the plurality of solid state battery cells being operable at a state of charge.

19. The device of claim 18 wherein the plurality of battery cells is wound or stacked.

20. The method of claim 17 wherein the numerical method is used for analysis of multiphysics problems in which partial or whole differential equations are solved simultaneously.

21. The method of claim 17 wherein the numerical method is selected from a finite element method, a finite element method (FEM), a finite difference method (FDM), a boundary element analysis, element-free Galerkin (EFG) or Smoothed Particle Hydrodynamics (SPH) method.

22. The method of claim 17 wherein the numerical method employs meshes or representations of surfaces and volumes.

23. The method of claim 17 wherein the one or more first characteristics comprise physical, electrical, thermal, mechanical, optical, or chemical characteristics.

24. The method of claim 23 wherein physical characteristics comprise but not limited to mass density, crystal structure, stoichiometry, ionic conductivity, diffusivity, moisture vapor transmission rate (MVTR), water vapor transmission rate (WVTR), and oxygen transmission rate (OTR).

25. The method of claim 23 wherein mechanical characteristics comprise but not limited to modulus, hardness, thermal expansion coefficient, and concentration expansion coefficient.

26. The method of claim 23 wherein electrical characteristics comprise but not limited to electronic conductivity, dielectric constant, sheet resistance, and contact resistance.

27. The method of claim 23 wherein thermal characteristics comprise but not limited to thermal conductivity, specific heat, melting temperature, vaporizing temperature.

28. The method of claim 23 wherein optical characteristics comprise but not limited to reflectance.

29. The method of claim 23 wherein chemical characteristics comprise but not limited to reaction constant, open circuit potential.

30. The method of claim 17 wherein the one or more second characteristics comprise layer thickness, layer width, layer length, layer spacing, interfacial interaction of connected layers, shape of each layer, defect size, defect distribution, defect material, type of layer materials, or electrochemical equilibrium or dynamic load considerations.

31. The method of claim 30 wherein the shape of each layer comprises flat, periodic patterned, or irregular shape, or combinations of these, and shape of each layer is independent of other layers.

32. The method of claim 17 wherein the performance parameters comprises lifetime, safety/physical/mechanical/chemical/thermal/ion concentration, voltage profile, state of charge, degree of intercalation, degree of achievable capacity under various discharge rate or discharge profile, intercalation-induced stresses, or volume changes.

33. The method of claim 17 wherein the layer of three dimensional electrochemical cell is selected from homogenous materials, inhomogenous materials or graded materials, or any combination of these.

34. The method of claim 33 wherein the graded materials comprise variation in composition and material structure over the volume of the layer.

35. The method of claim 34 wherein material structure comprise crystalline structure, or amorphous structure, or any combination of these.

36. A computer-aided system for processing information related to a multi-layered solid-state battery device, the system comprising one or more computer readable

memory, the one or more computer readable memory comprising: one or more computer codes for outputting a computer generated relationship between one or more first characteristics referenced against one or more second characteristics for a selected material set for a design of three dimensional spatial elements in a three- dimensional electrochemical cell; one or more codes directed to selecting one or more of the first characteristics or second characteristics for the selected material set; one or more codes directed to processing the one or more selected first or second characteristics to determine whether the one or more first or second characteristics is within one or more predetermined performance parameters; and one or more codes directed to executing a program for processing the one or more first characteristics or second characteristics to provide the three dimensional electrochemical cell.

37. The method of claim 36 wherein a multi-layered solid-state battery device comprising a plurality of solid state battery cells numbered from 1 through N, each of the solid state battery cells comprising a first current collector overlying the substrate member, a cathode device overlying the first current collector, an electrolyte device overlying the first current collector, an anode device overlying the electrolyte device, and a second current collector overlying the anode device, each of the plurality of solid state battery cells being operable at a state of charge.

38. The device of claim 37 wherein the plurality of battery cells is wound or stacked.

39. The method of claim 36 wherein the one or more first characteristics comprise physical, electrical, thermal, mechanical, optical, or chemical characteristics.

40. The method of claim 39 wherein physical characteristics comprise but not limited to mass density, crystal structure, stoichiometry, ionic conductivity, diffusivity, moisture vapor transmission rate (MVTR), water vapor transmission rate (WVTR), and oxygen transmission rate (OTR)

41. The method of claim 39 wherein mechanical characteristics comprise but not limited to modulus, hardness, thermal expansion coefficient, and concentration expansion coefficient.

42. The method of claim 39 wherein electrical characteristics comprise but not limited to electronic conductivity, dielectric constant, sheet resistance, and contact resistance.

43. The method of claim 39 wherein thermal characteristics comprise but not limited to thermal conductivity, specific heat, melting temperature, vaporizing temperature.

44. The method of claim 39 wherein optical characteristics comprise but not limited to reflectance.

45. The method of claim 39 wherein chemical characteristics comprise but not limited to reaction constant, open circuit potential.

46. The method of claim 36 wherein the one or more second characteristics comprise layer thickness, layer width, layer length, layer spacing, interfacial interaction of connected layers, shape of each layer, defect size, defect distribution, defect material, type of layer materials, or electrochemical equilibrium or dynamic load considerations.

47. The method of claim 46 wherein the shape of each layer comprises flat, periodic patterned, or irregular shape, or combinations of these, and shape of each layer is independent of other layers.

48. The method of claim 36 wherein the performance parameters comprises lifetime, safety/physical/mechanical/chemical/thermal/ion concentration, voltage profile, state of charge, degree of intercalation, degree of achievable capacity under various discharge rate or discharge profile, intercalation-induced stresses, or volume changes.

49. The method of claim 36 wherein the layer of three dimensional electrochemical cell is selected from homogenous materials, inhomogenous materials or graded materials, or any combination of these.

50. The method of claim 49 wherein the graded materials comprise variation in composition and material structure over the volume of the layer.

51. The method of claim 50 wherein material structure comprise crystalline structure, or amorphous structure, or any combination of these.

52. The system of claim 36 further comprising one or more codes directed to a post processing program.

53. The system of claim 36 further comprising one or more codes directed to a meshing program.

54. The system of claim 36 further comprising one or more codes directed to one or more boundary conditions.

55. The system of claim 36 further comprising one or more codes directed to one or more irregular shaped objects, the one or more irregular shaped objects associated with one or more of the second characteristics.

56. A method for manufacturing a multi-layered solid-state battery device, the method comprising: generating spatial information each layer geometry; storing the spatial information including each layer geometry into a database structure; selecting one or more material properties from a plurality of materials; using the one or more material properties with the spatial information in a simulation program; and outputting one or more performance parameters from the simulation program.

57. The method of claim 56 wherein a multi-layered solid-state battery device comprising a plurality of solid state battery cells numbered from 1 through N, each of the

solid state battery cells comprising a first current collector overlying the substrate member, a cathode device overlying the first current collector, an electrolyte device overlying the first current collector, an anode device overlying the electrolyte device, and a second current collector overlying the anode device, each of the plurality of solid state battery cells being operable at a state of charge.

58. The device of claim 56 wherein the plurality of battery cells is wound or stacked.

59. The method of claim 56 wherein the one or more material properties is selected from physical, electrical, thermal, mechanical, optical, or chemical characteristics.

60. The method of claim 59 wherein physical characteristics comprise but not limited to mass density, crystal structure, stoichiometry, ionic conductivity, diffusivity, moisture vapor transmission rate (MVTR), water vapor transmission rate (WVTR), and oxygen transmission rate (OTR).

61. The method of claim 59 wherein mechanical characteristics comprise but not limited to modulus, hardness, thermal expansion coefficient, and concentration expansion coefficient.

62. The method of claim 59 wherein electrical characteristics comprise but not limited to electronic conductivity, dielectric constant, sheet resistance, and contact resistance.

63. The method of claim 59 wherein thermal characteristics comprise but not limited to thermal conductivity, specific heat, melting temperature, vaporizing temperature.

64. The method of claim 59 wherein optical characteristics comprise but not limited to reflectance.

65. The method of claim 59 wherein chemical characteristics comprise but not limited to reaction constant, open circuit potential.

66. The method of claim 56 further comprising selecting one or more other material properties from the plurality of materials and repeating the using, outputting, and processing steps until the one or more performance parameters are within a tolerance of the one or more desired performance parameters.

67. The method of claim 56 wherein the spatial information includes layer shape, shape, spatial orientation, or other spatial information.

68. The method of claim 56 wherein the spatial information is selected from a stacked configuration, an inter-digitated configuration, or a sinusoidal configuration.

69. The method of claim 56 wherein the simulation progress uses at least a finite element process.

70. The method of claim 56 wherein the spatial information comprises a plurality of irregularly shaped objects, the irregularly shaped objects are selected from fibers, pellets, disks, spheres, and ellipsoids, and mixtures of any of them.

71. The method of claim 56 wherein the spatial information comprises intrinsic information and extrinsic information.

72. The method of claim 56 wherein the performance parameters comprises lifetime, safety/physical/mechanical/chemical/thermal/ion concentration, voltage profile, state of charge, degree of intercalation, degree of achievable capacity under various discharge rate or discharge profile, intercalation-induced stresses, or volume changes.

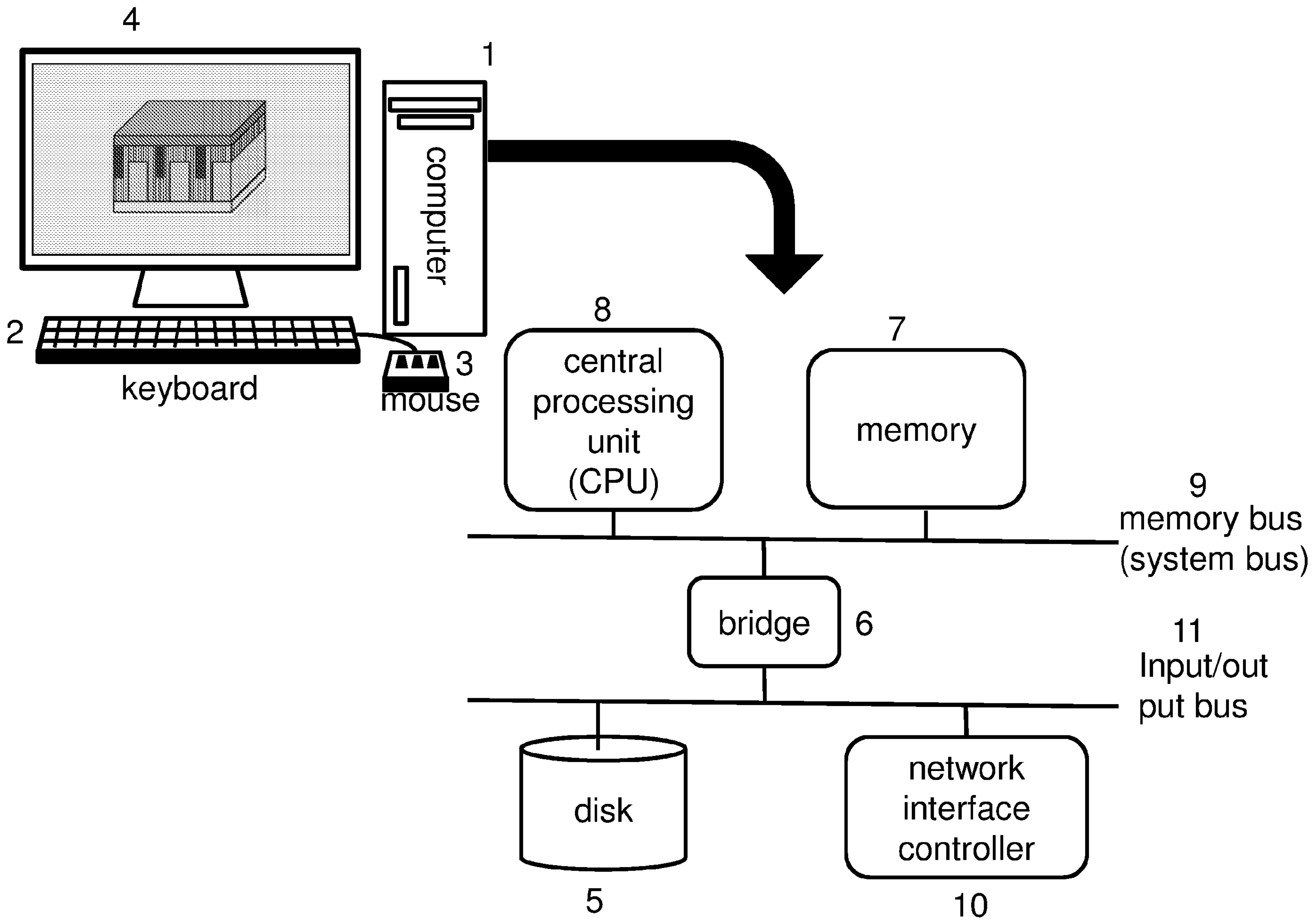

4
1
computer
2
keyboard
3
mouse
8
central processing unit (CPU)
7
memory
9
memory bus (system bus)
bridge
6
11
Input/output bus
disk
5
network interface controller
10

figure 1

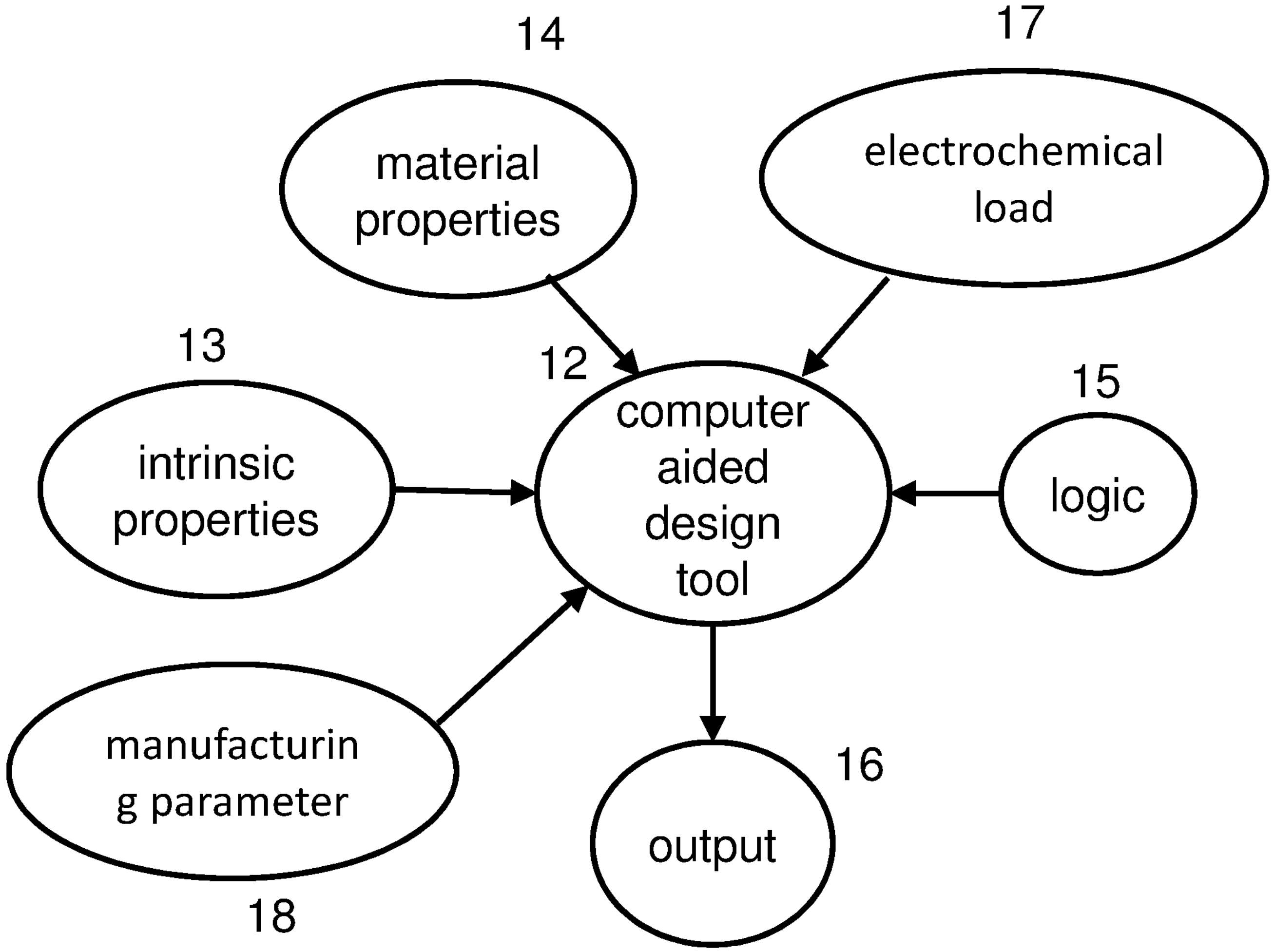

14
material properties
17
electrochemical load
13
intrinsic properties
12
computer aided design tool
15
logic
manufacturing parameter
18
16
output

figure 2

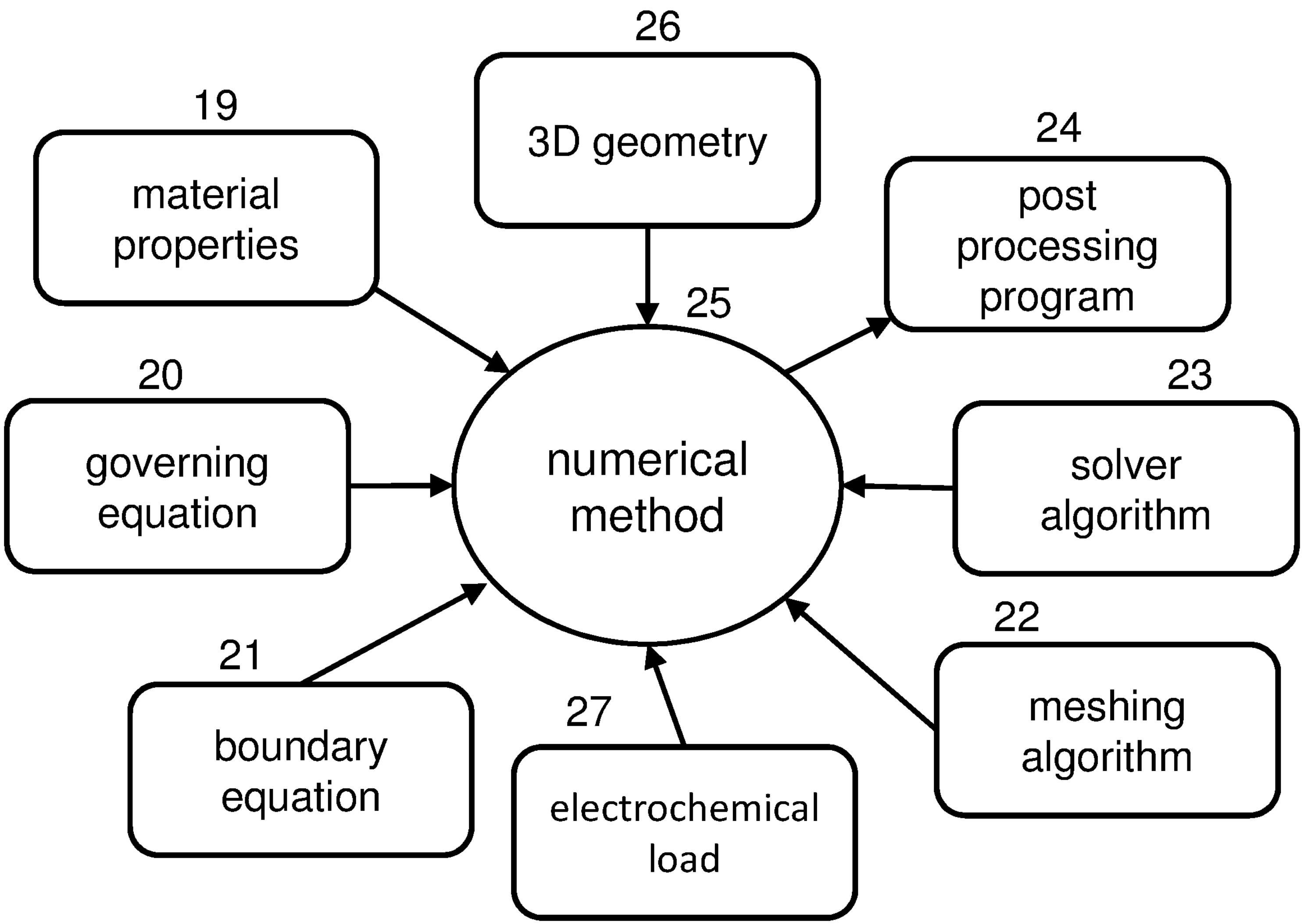

26
3D geometry
19
material properties
24
post processing program
25
numerical method
20
governing equation
23
solver algorithm
22
meshing algorithm
21
boundary equation
27
electrochemical load

figure 3

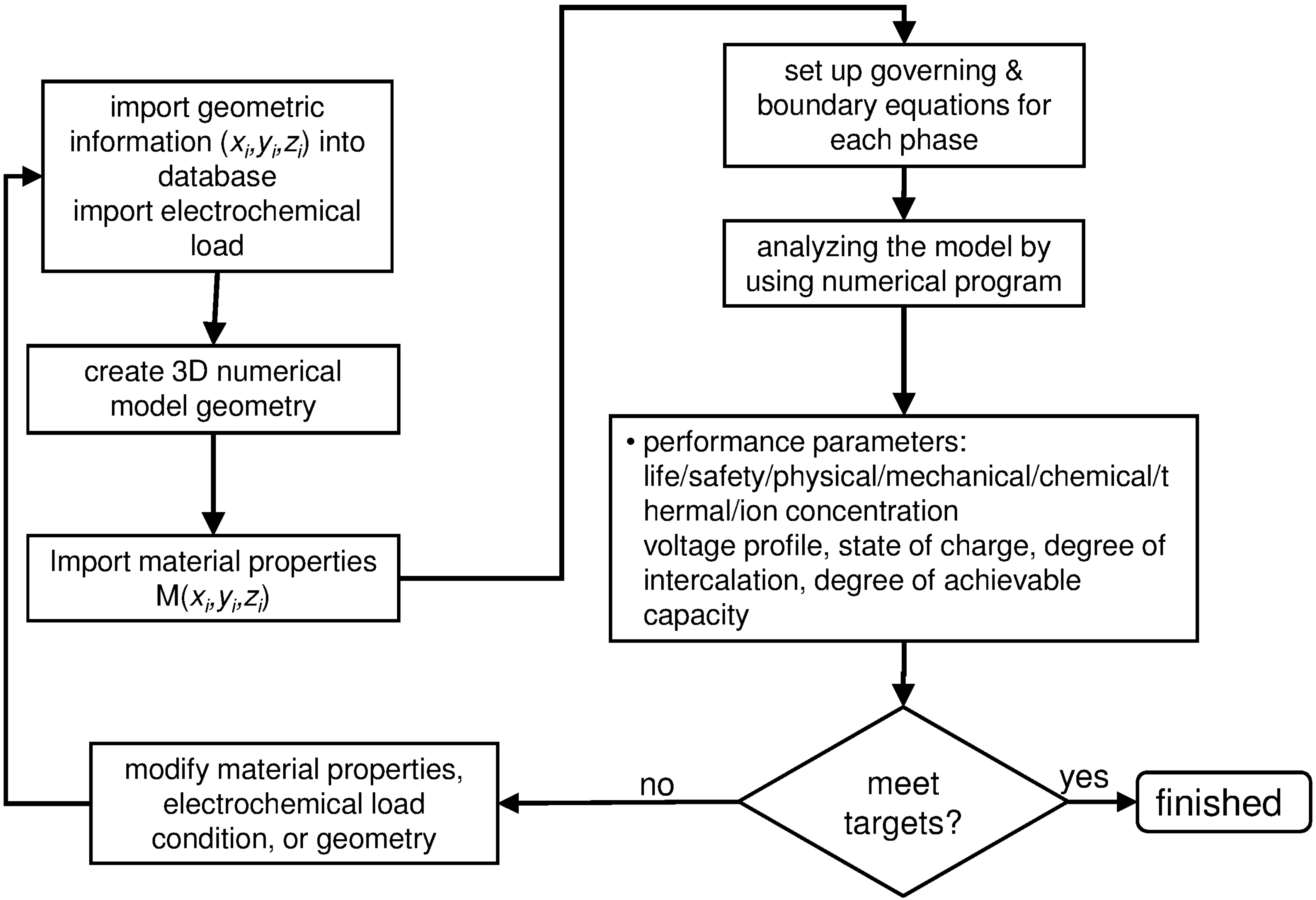

import geometric information (x_i,y_i,z_i) into database
import electrochemical load
create 3D numerical model geometry
Import material properties M(x_i,y_i,z_i)
set up governing & boundary equations for each phase
analyzing the model by using numerical program
• performance parameters:
life/safety/physical/mechanical/chemical/thermal/ion concentration
voltage profile, state of charge, degree of intercalation, degree of achievable capacity
meet targets?
yes
finished
no
modify material properties, electrochemical load condition, or geometry

figure 4

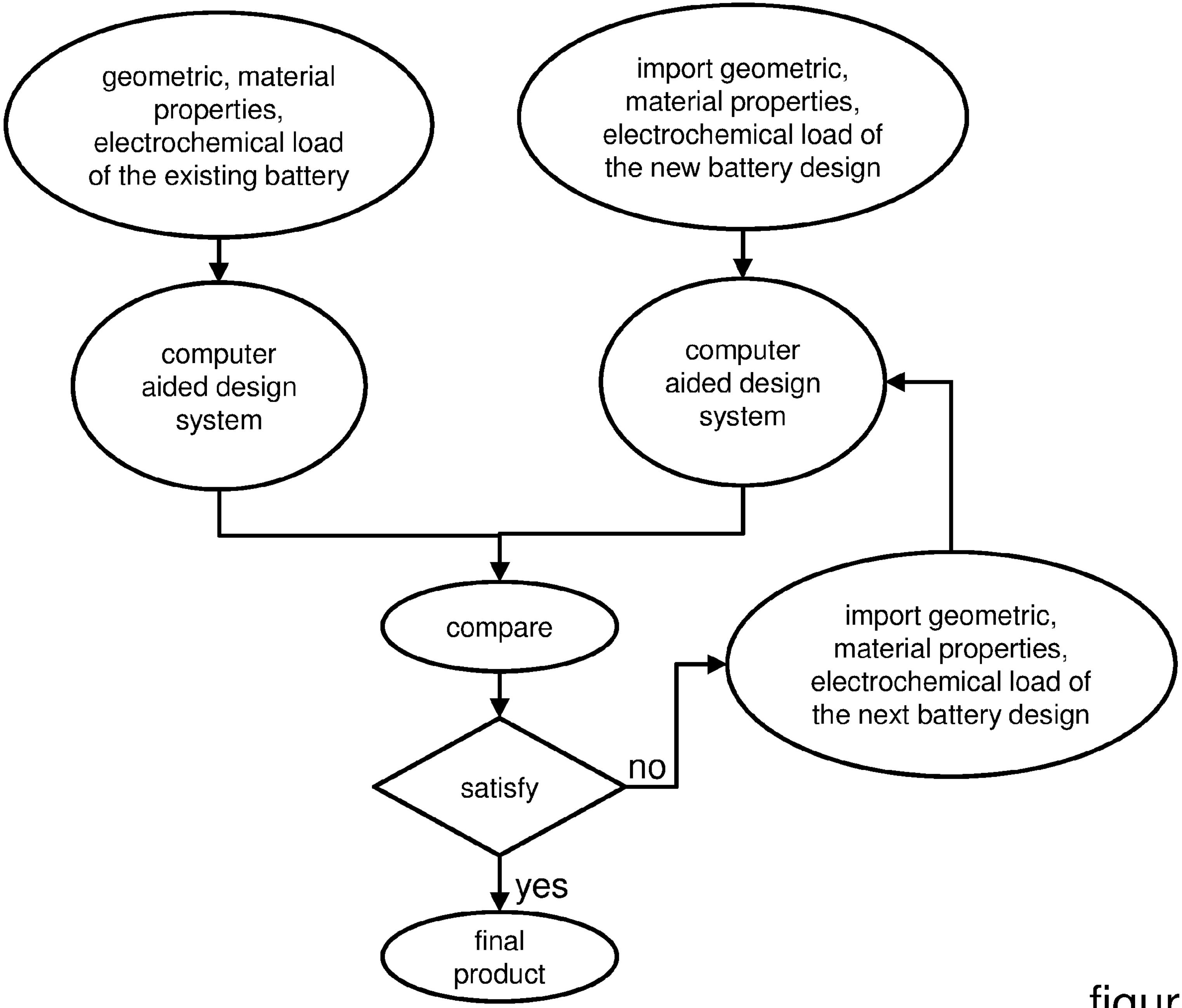

geometric, material properties, electrochemical load of the existing battery
import geometric, material properties, electrochemical load of the new battery design
computer aided design system
computer aided design system
compare
import geometric, material properties, electrochemical load of the next battery design
satisfy
no
yes
final product

figure 5A

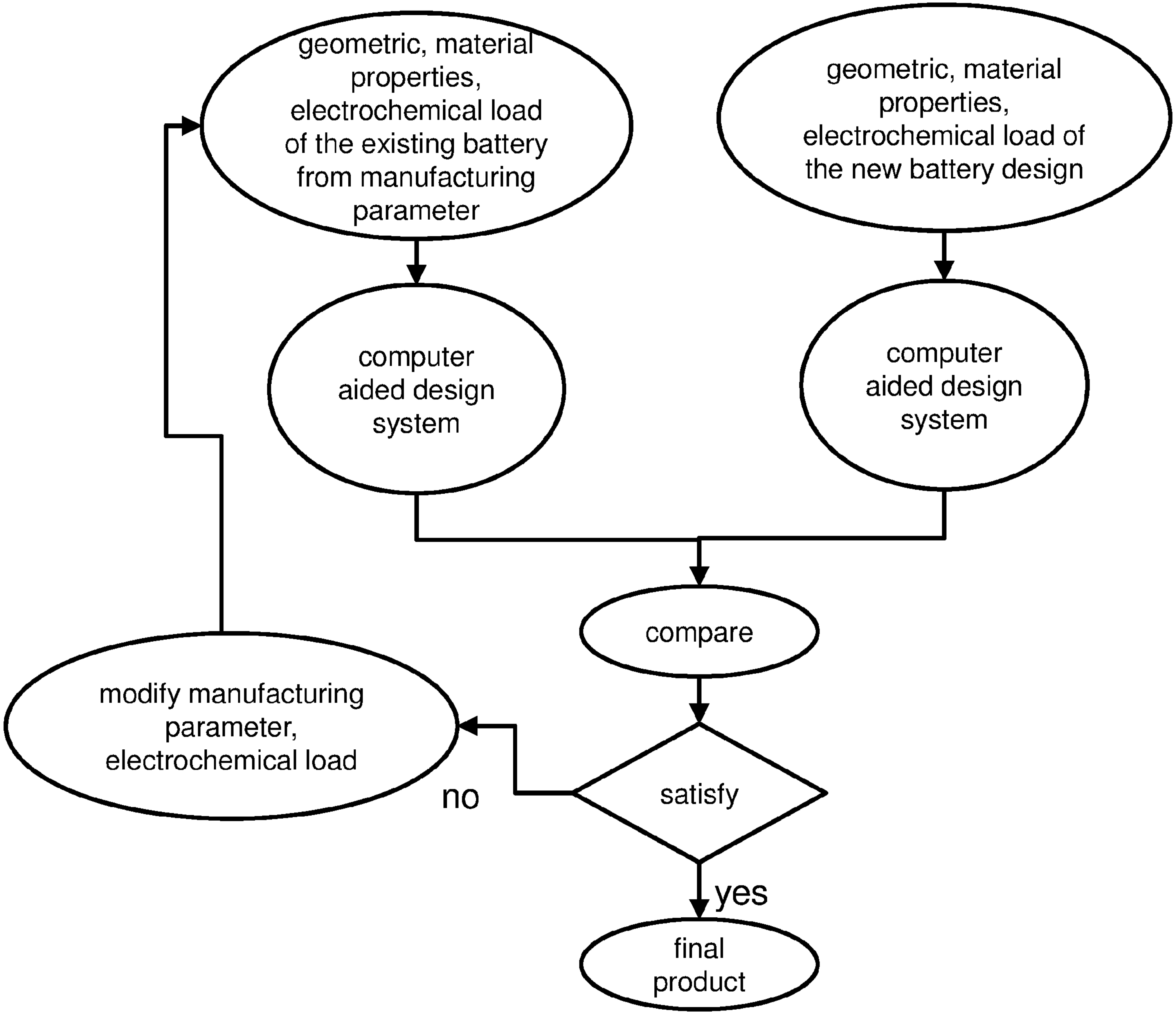

geometric, material properties, electrochemical load of the existing battery from manufacturing parameter
geometric, material properties, electrochemical load of the new battery design
computer aided design system
computer aided design system
compare
satisfy
no
yes
modify manufacturing parameter, electrochemical load
final product

figure 5B

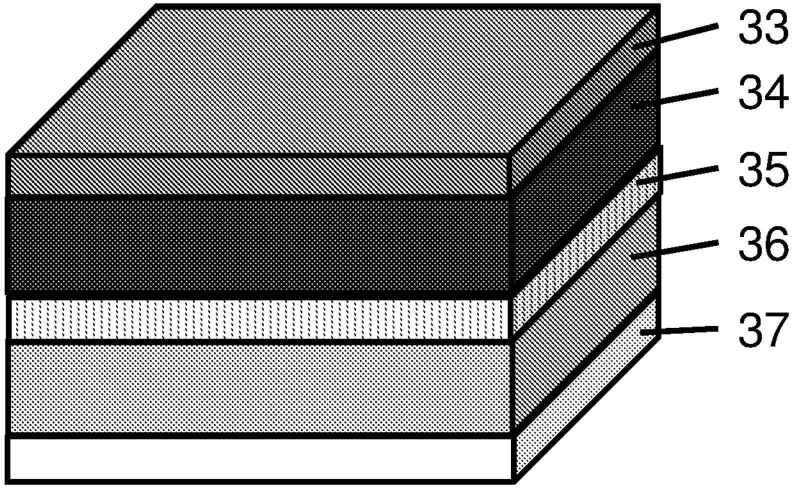


figure 6(A)

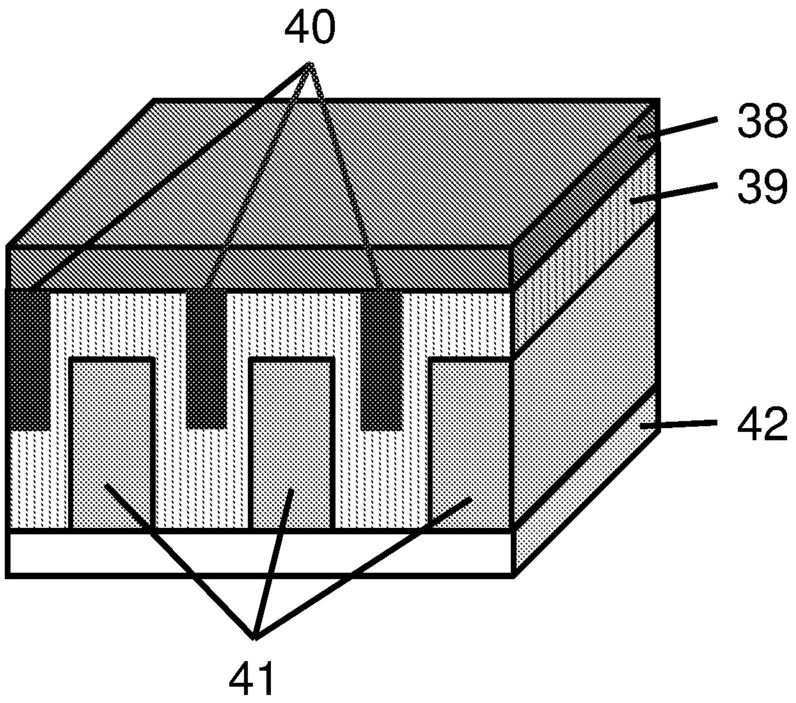


figure 6(B)

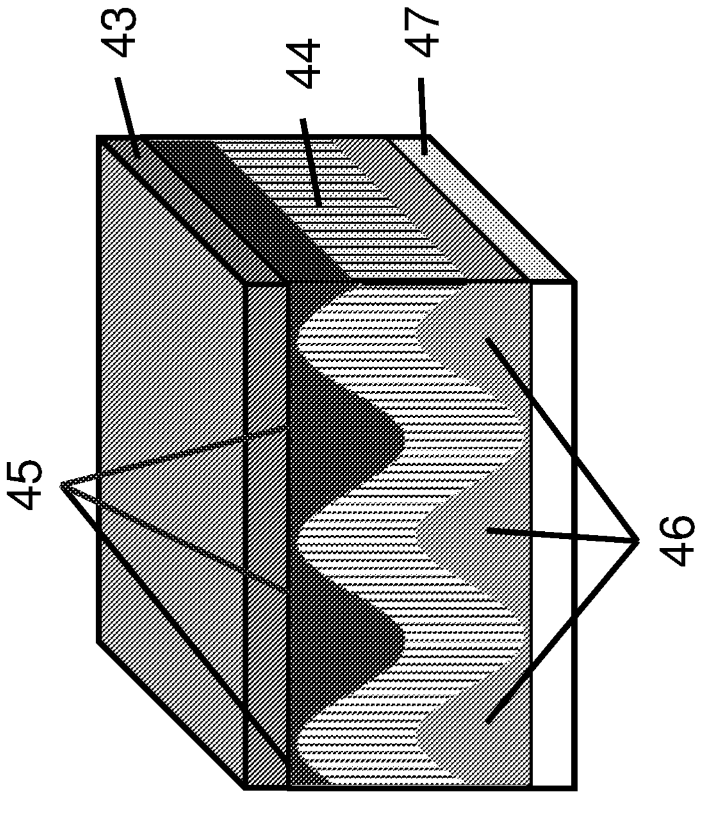
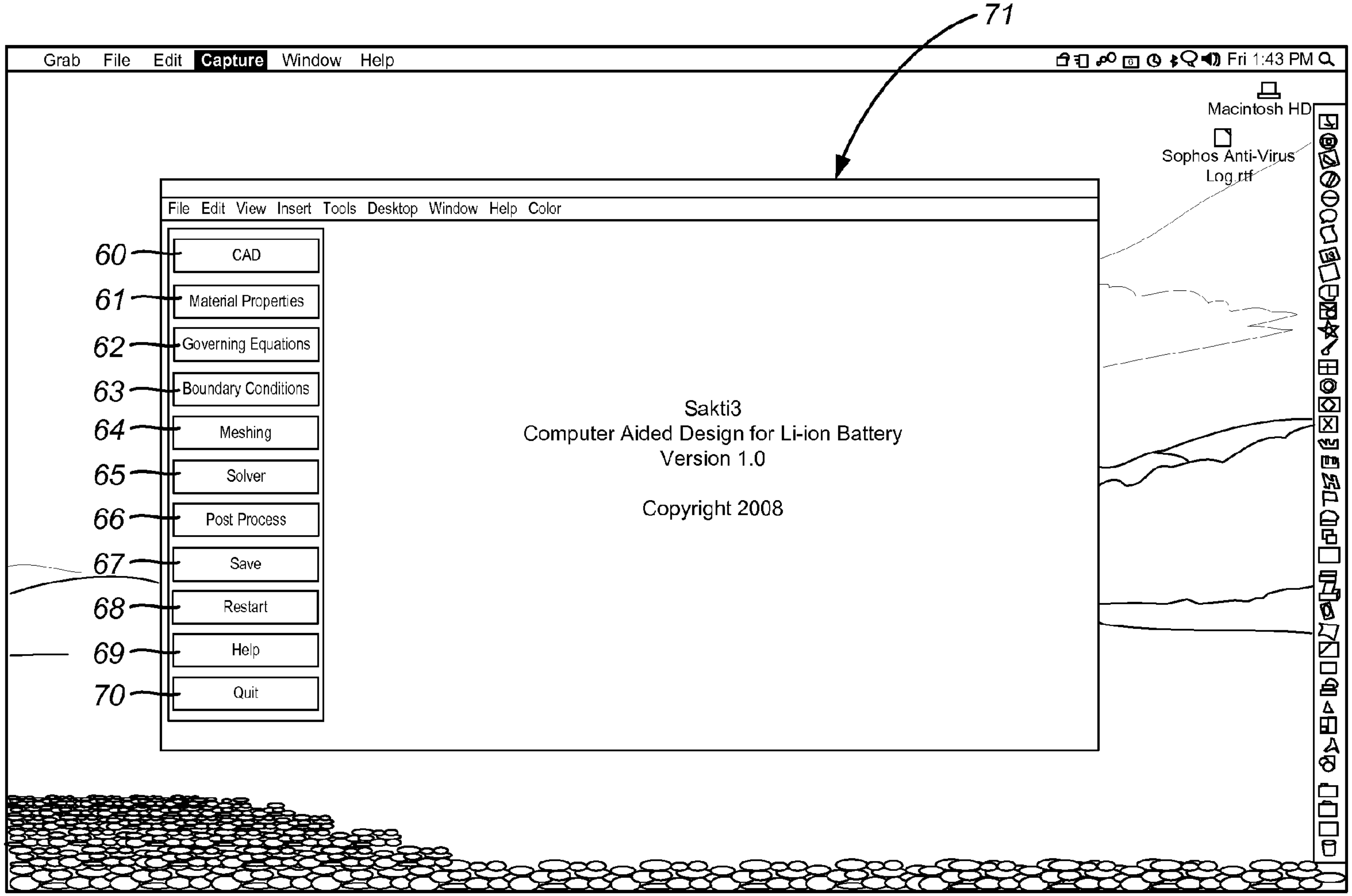


figure 6(C)



Sakti3
Computer Aided Design for Li-ion Battery
Version 1.0

Copyright 2008

figure 7(A)

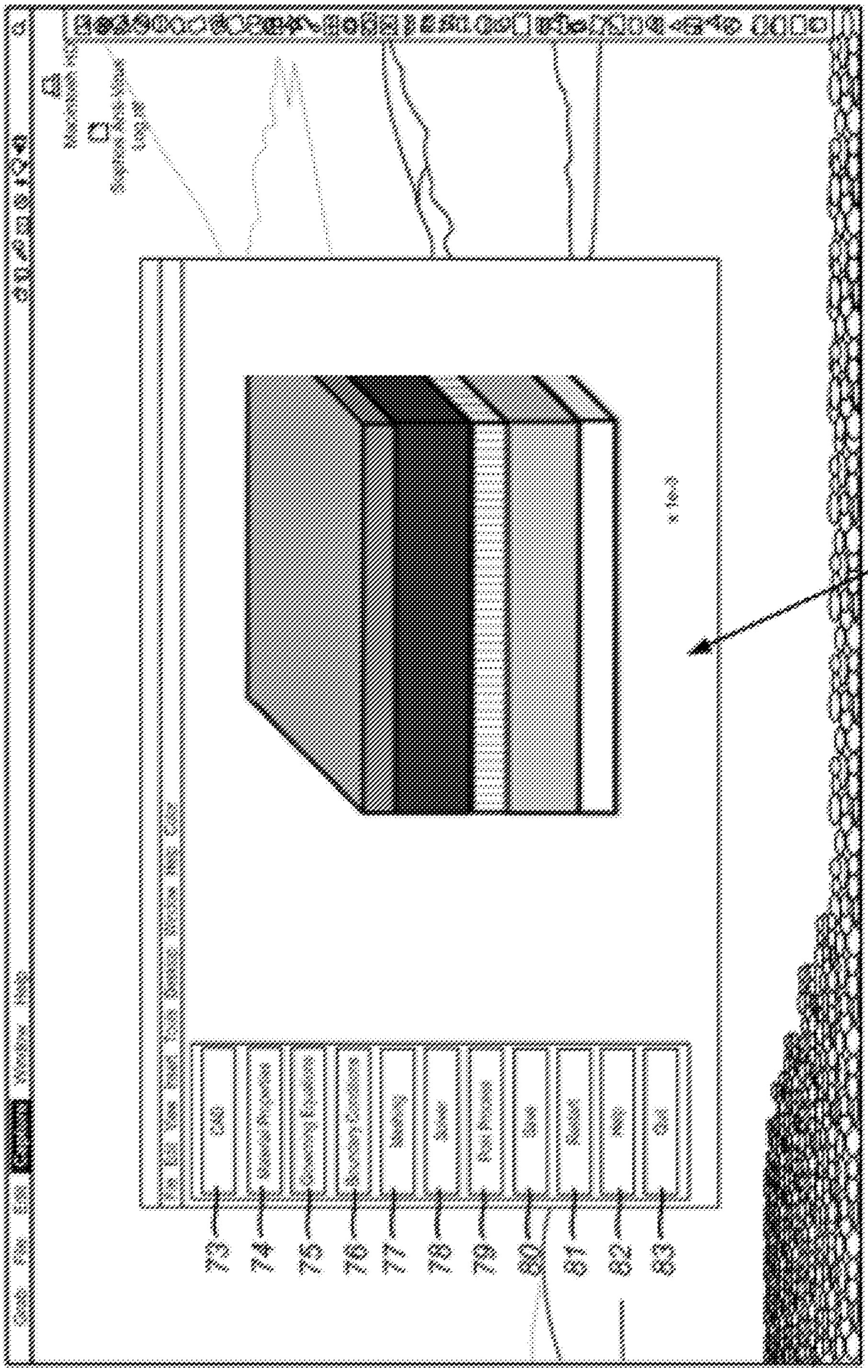


figure 7(B)

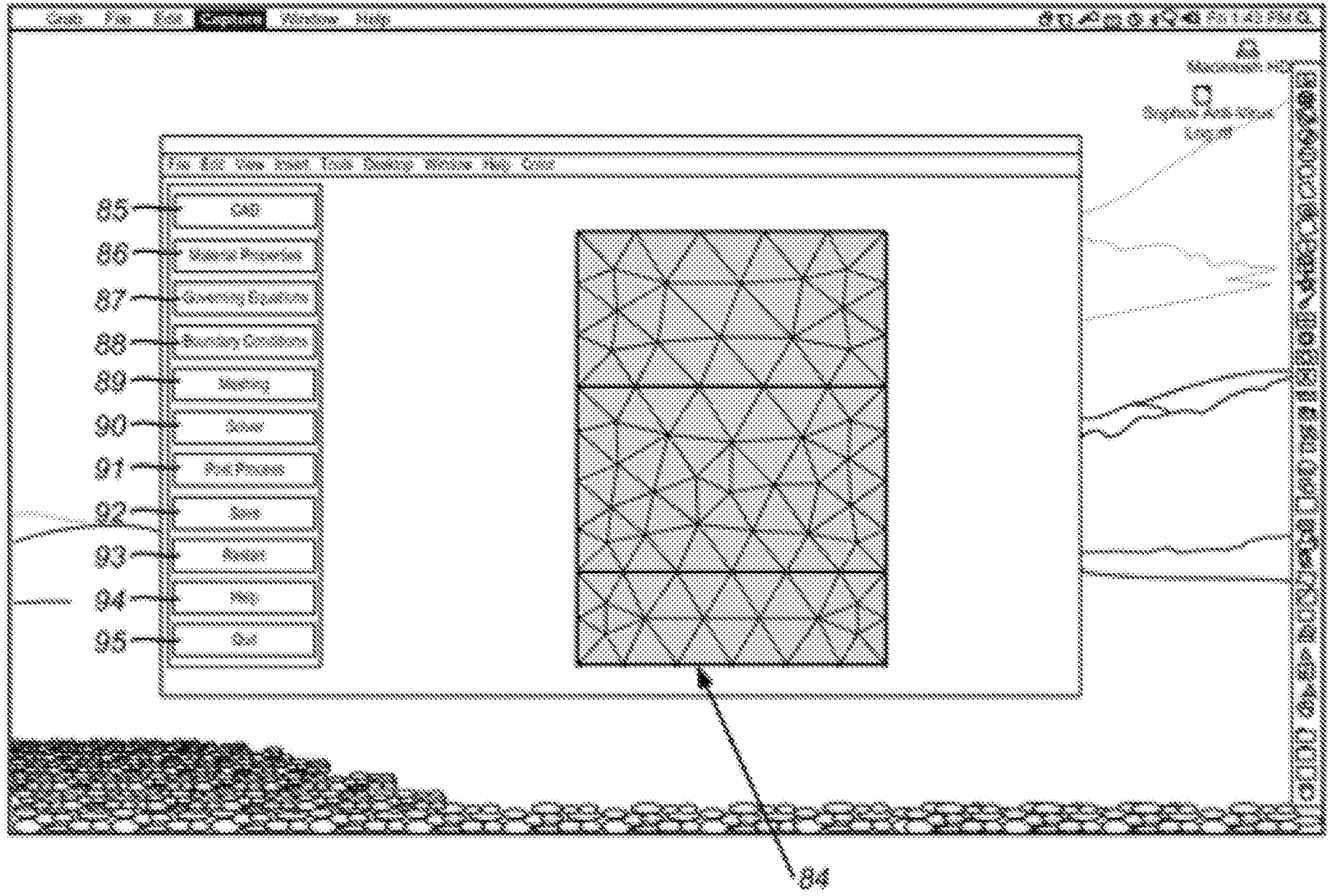


figure 7(C)

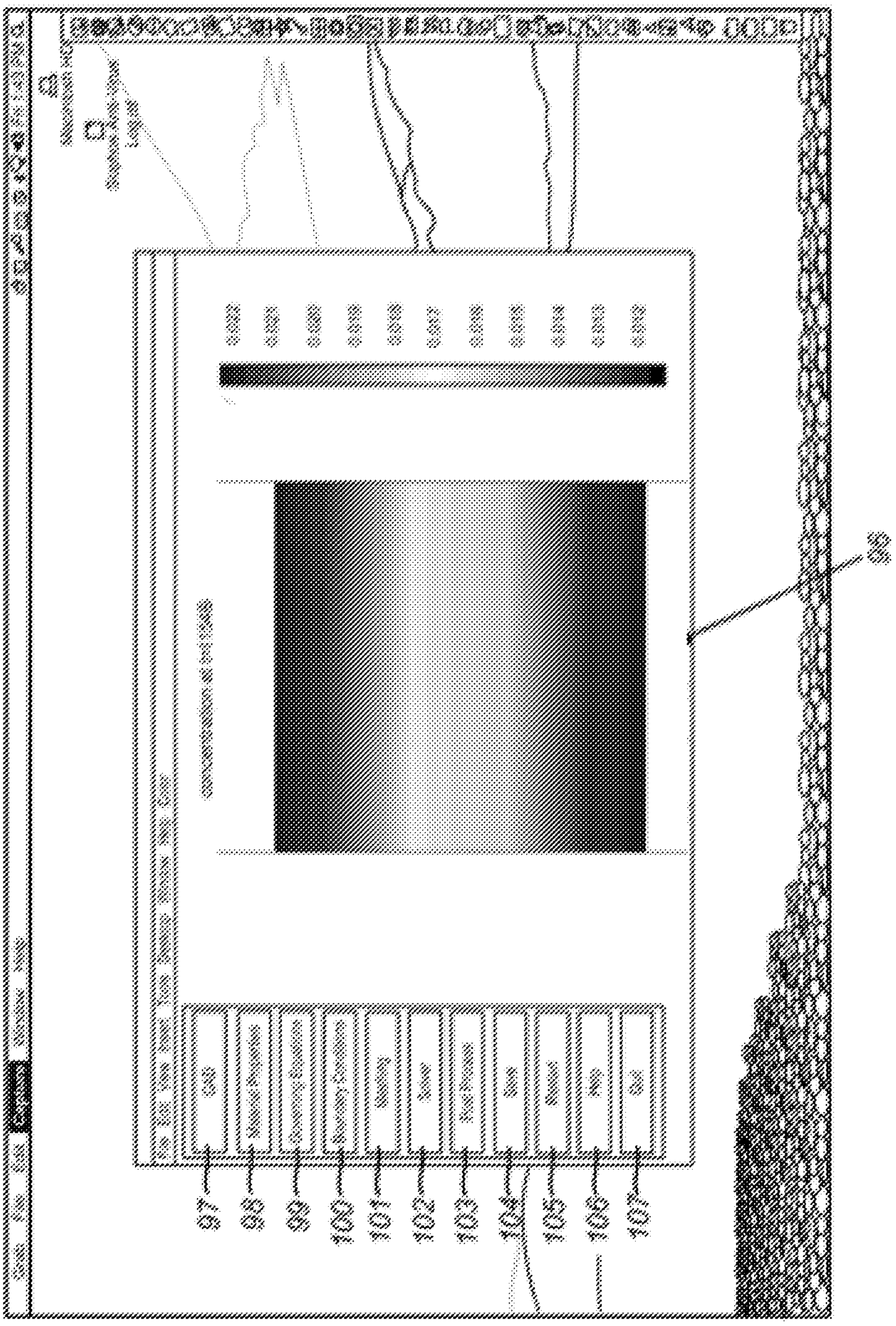


figure 7(D)

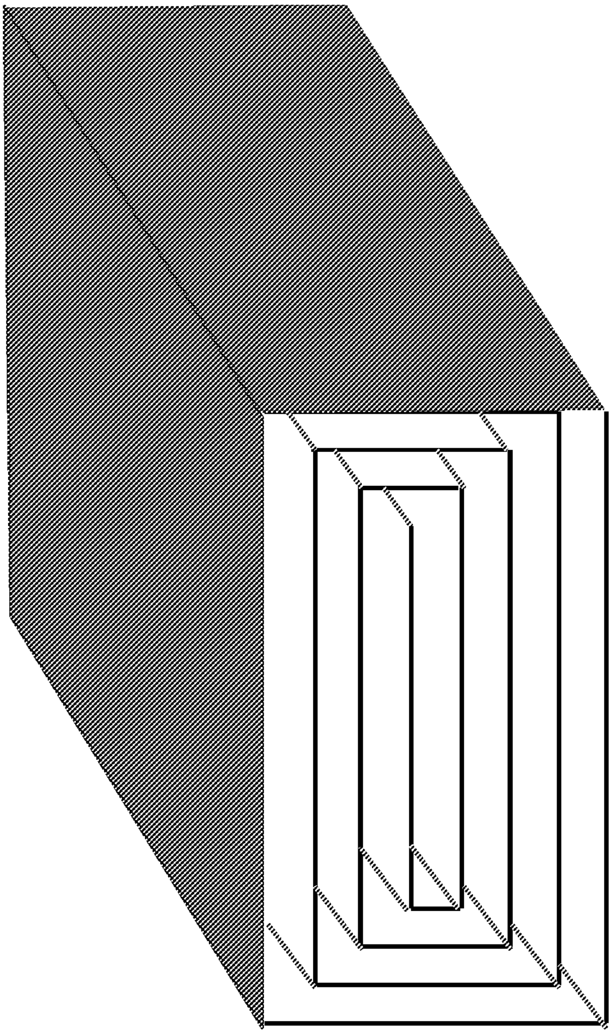
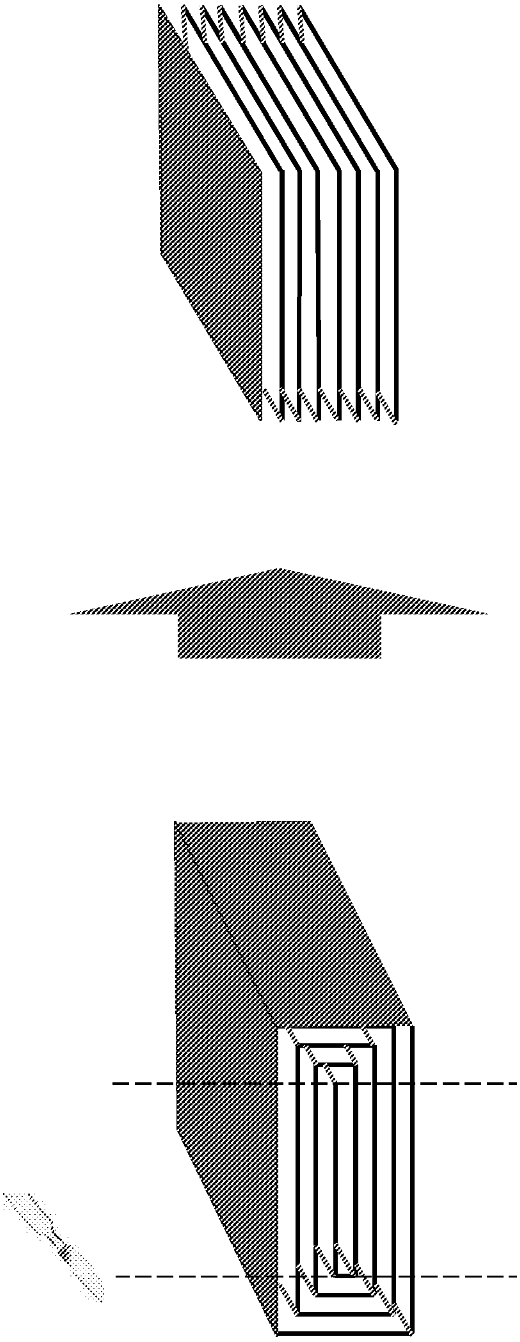


figure 8

figure 9



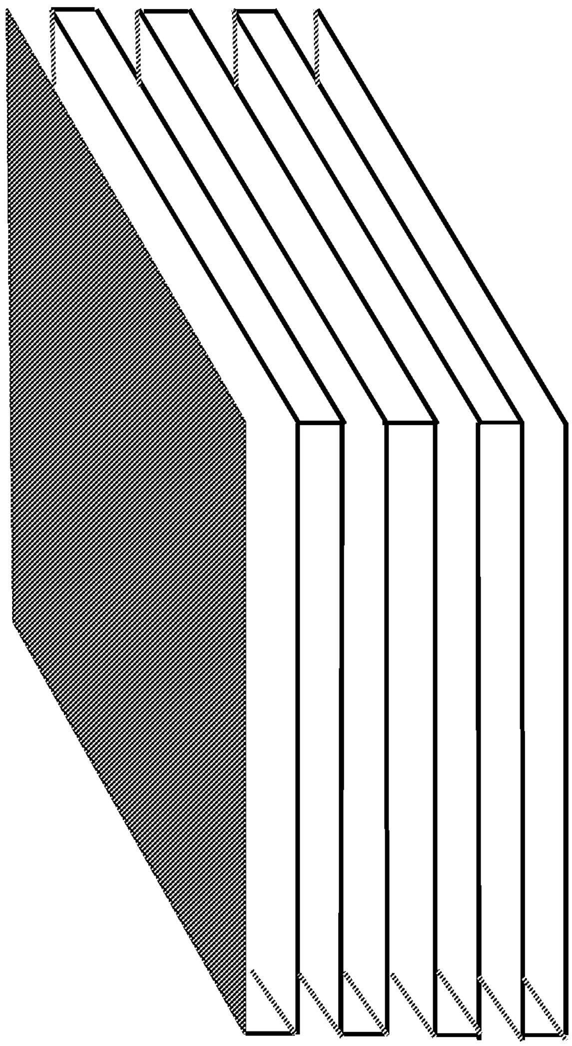


figure 10

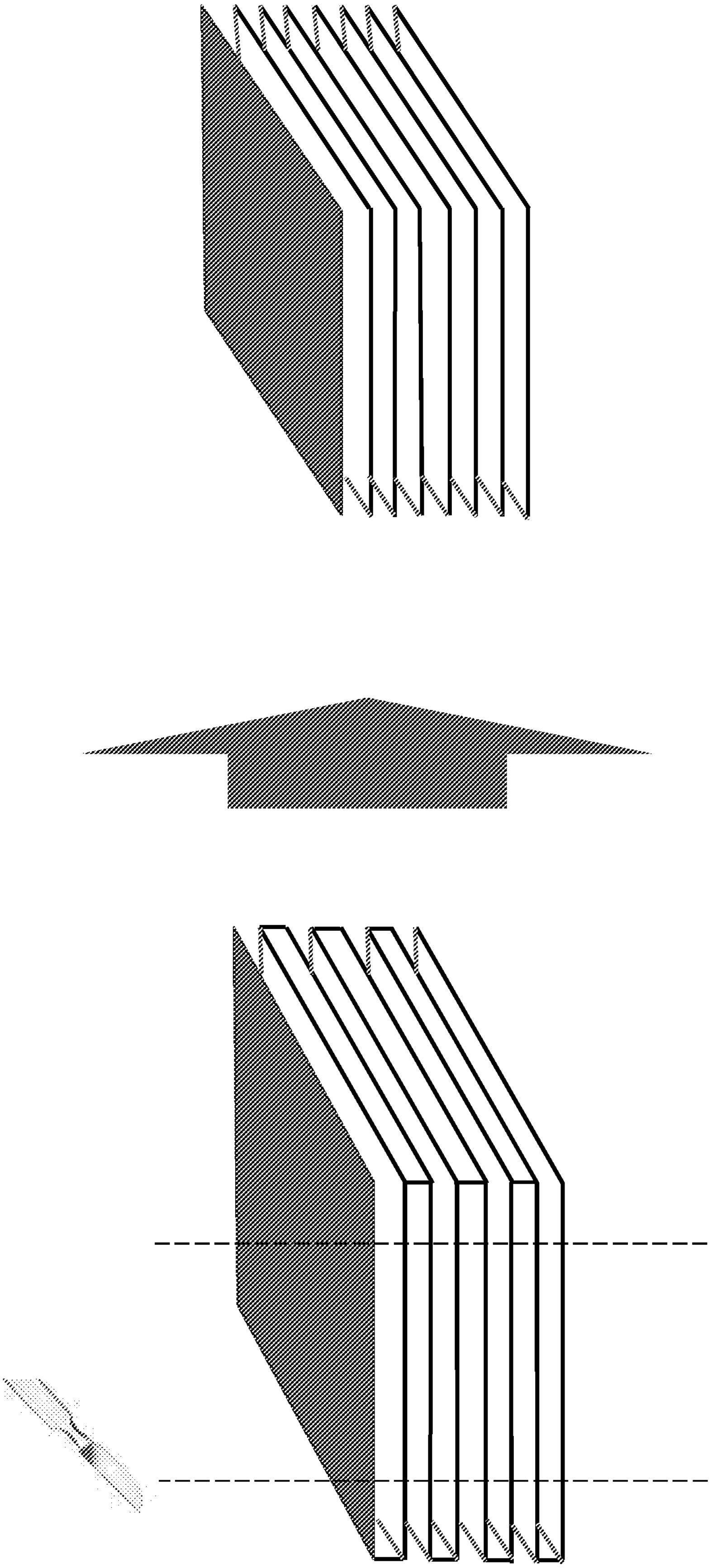


figure 11

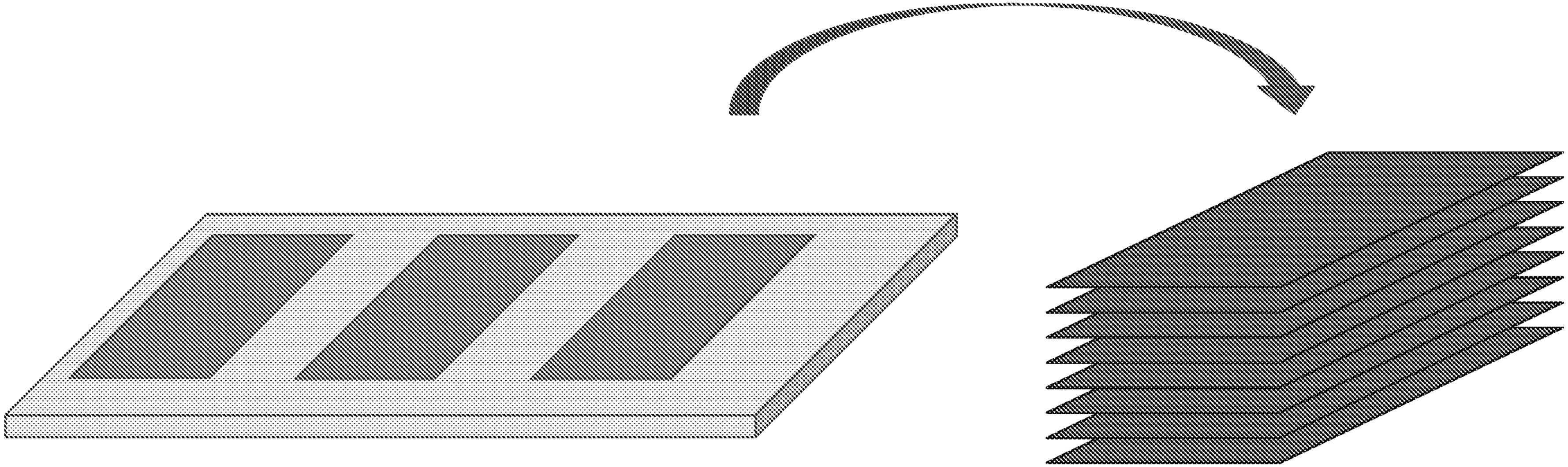


figure 12

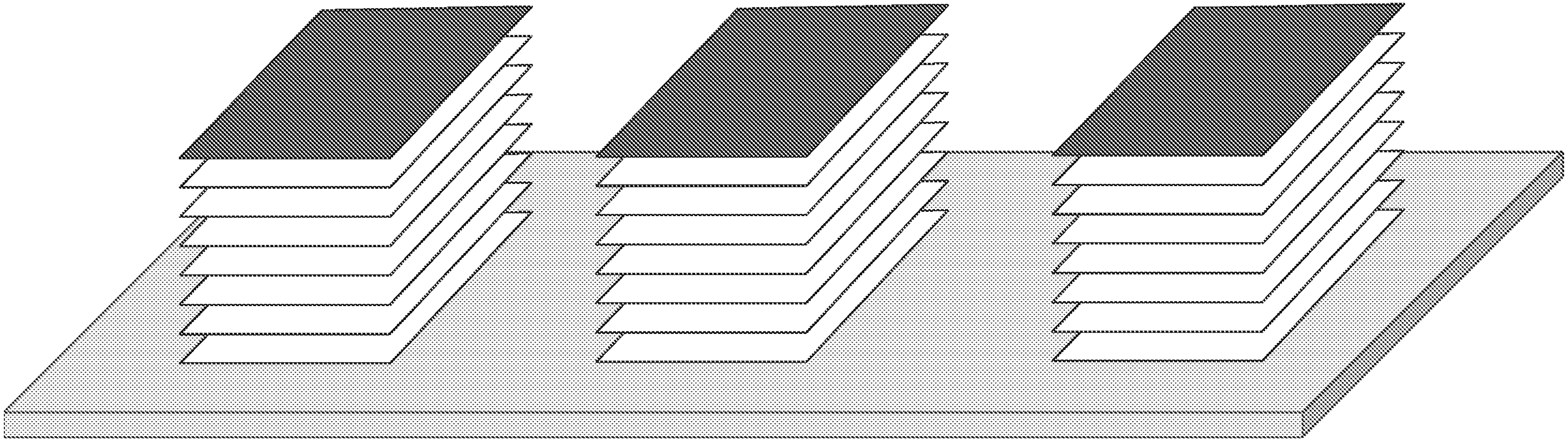


figure 13

contour plot of volumetric energy density (Wh/l) at different voltage cut-offs

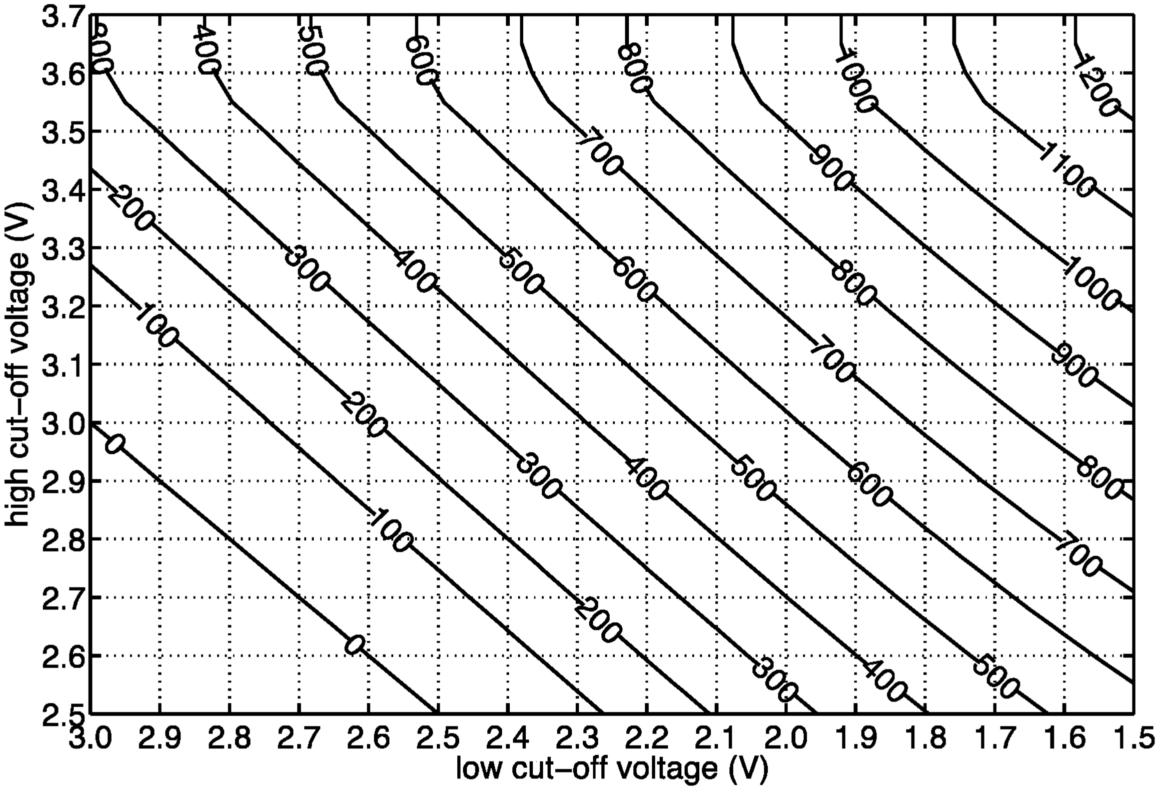
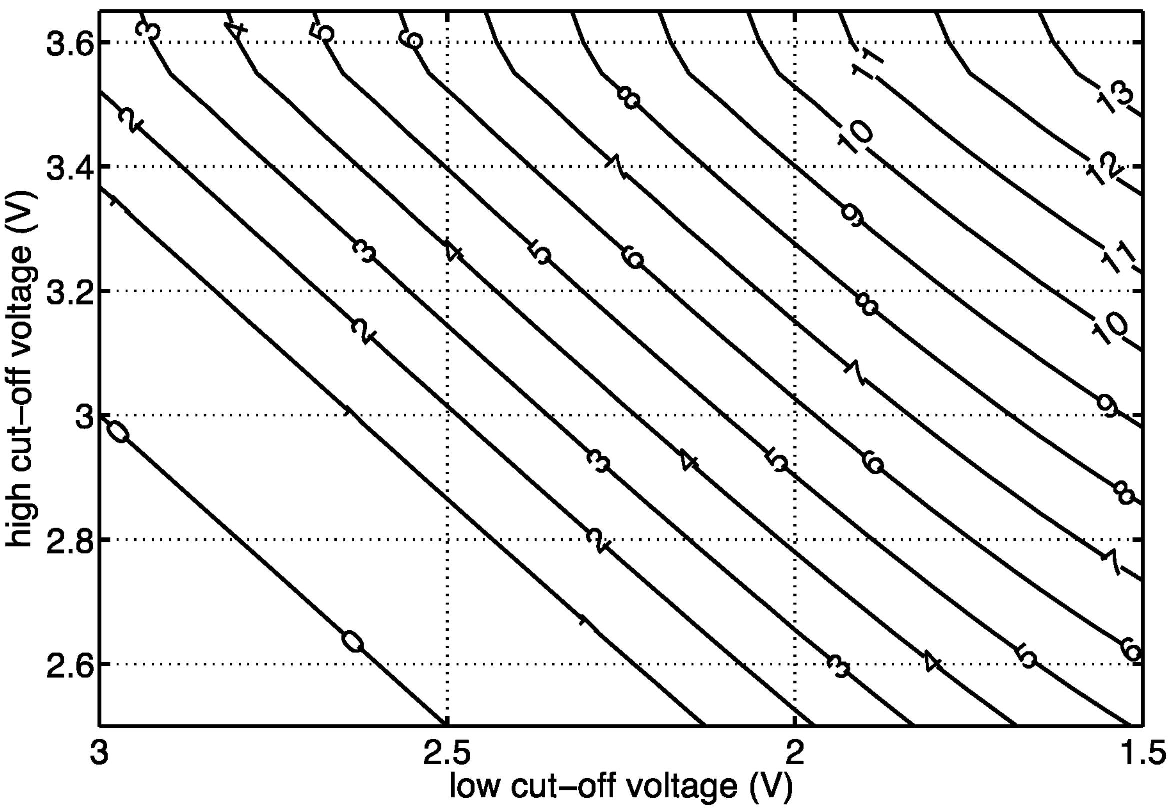


figure 14



contour plot of operational time (min) at different voltage cut-offs

figure 15

contour plot of operational time (min) at different voltage cut-offs

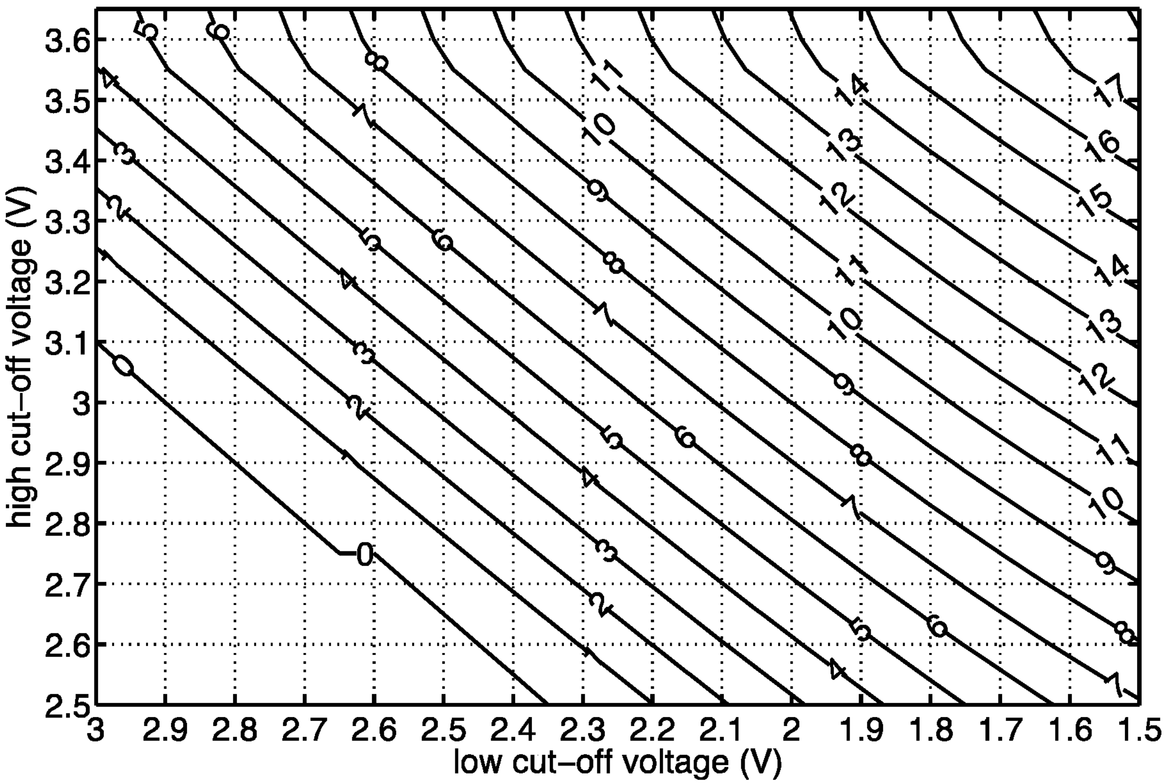


figure 16

contour plot of volumetric energy density (Wh/l) at different voltage cut-offs

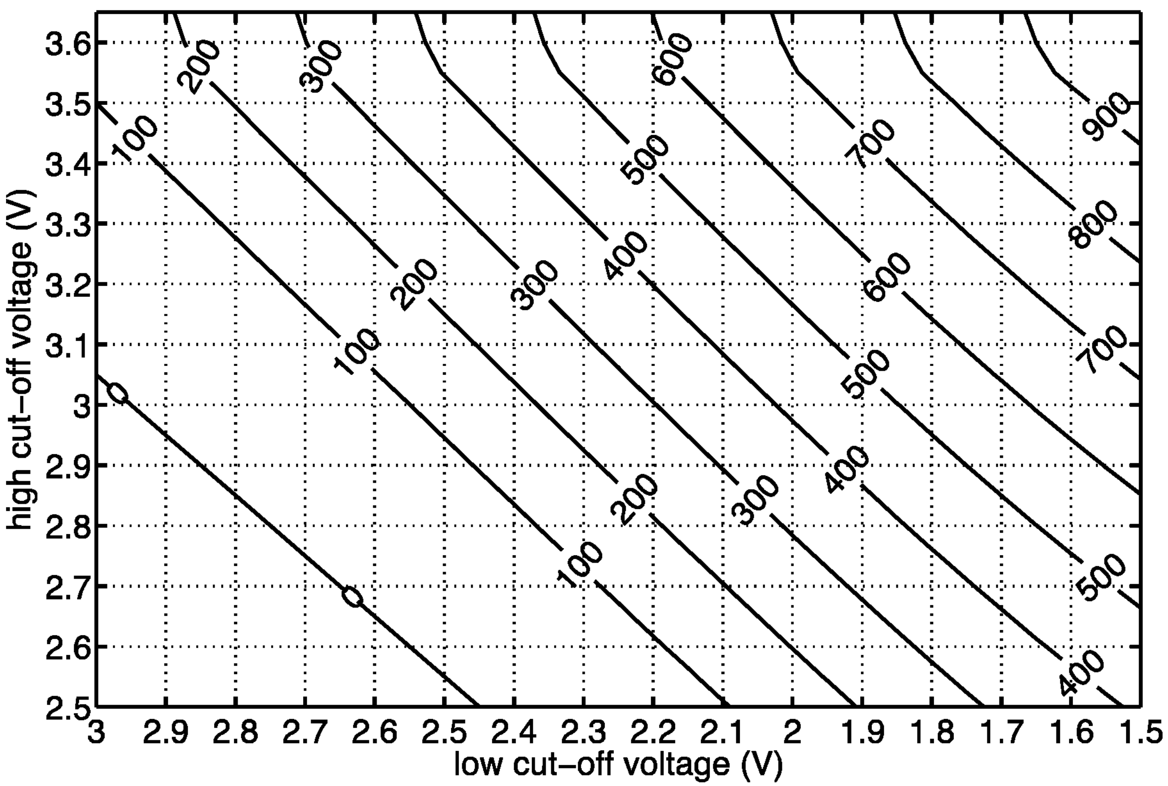


figure 17

contour plot of volumetric energy density (Wh/l) at different voltage cut-offs

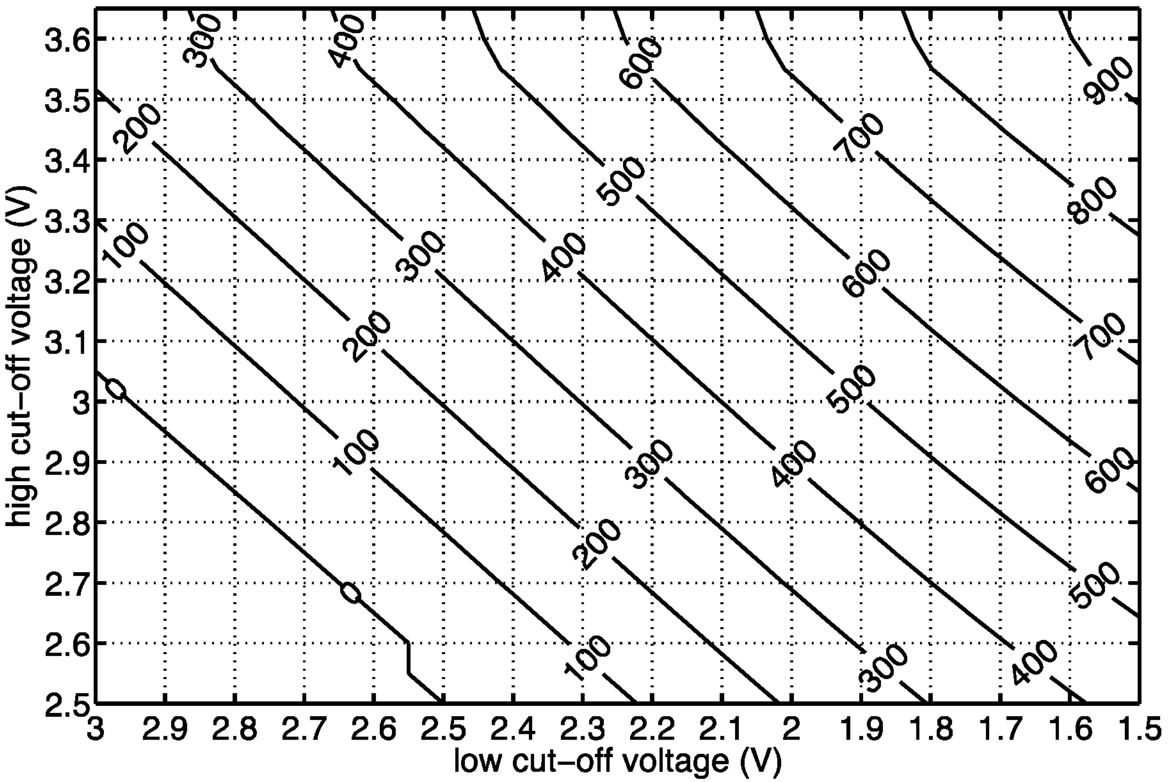


figure 18

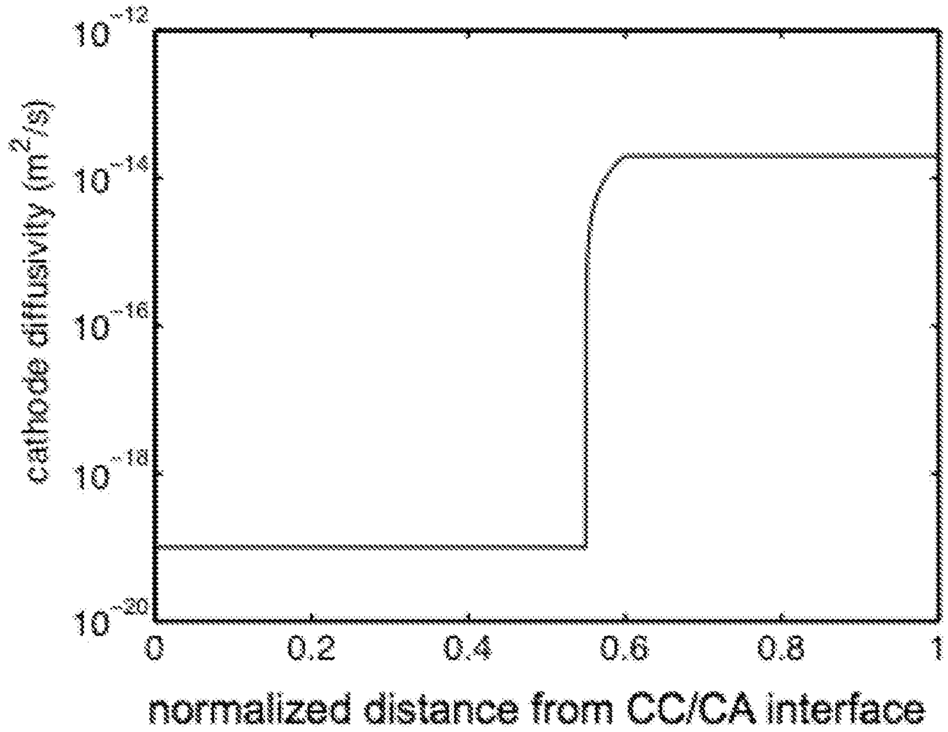

cathode diffusivity (m^2/s)
10^{-12}
10^{-14}
10^{-16}
10^{-18}
10^{-20}
0
0.2
0.4
0.6
0.8
1
normalized distance from CC/CA interface

figure 19

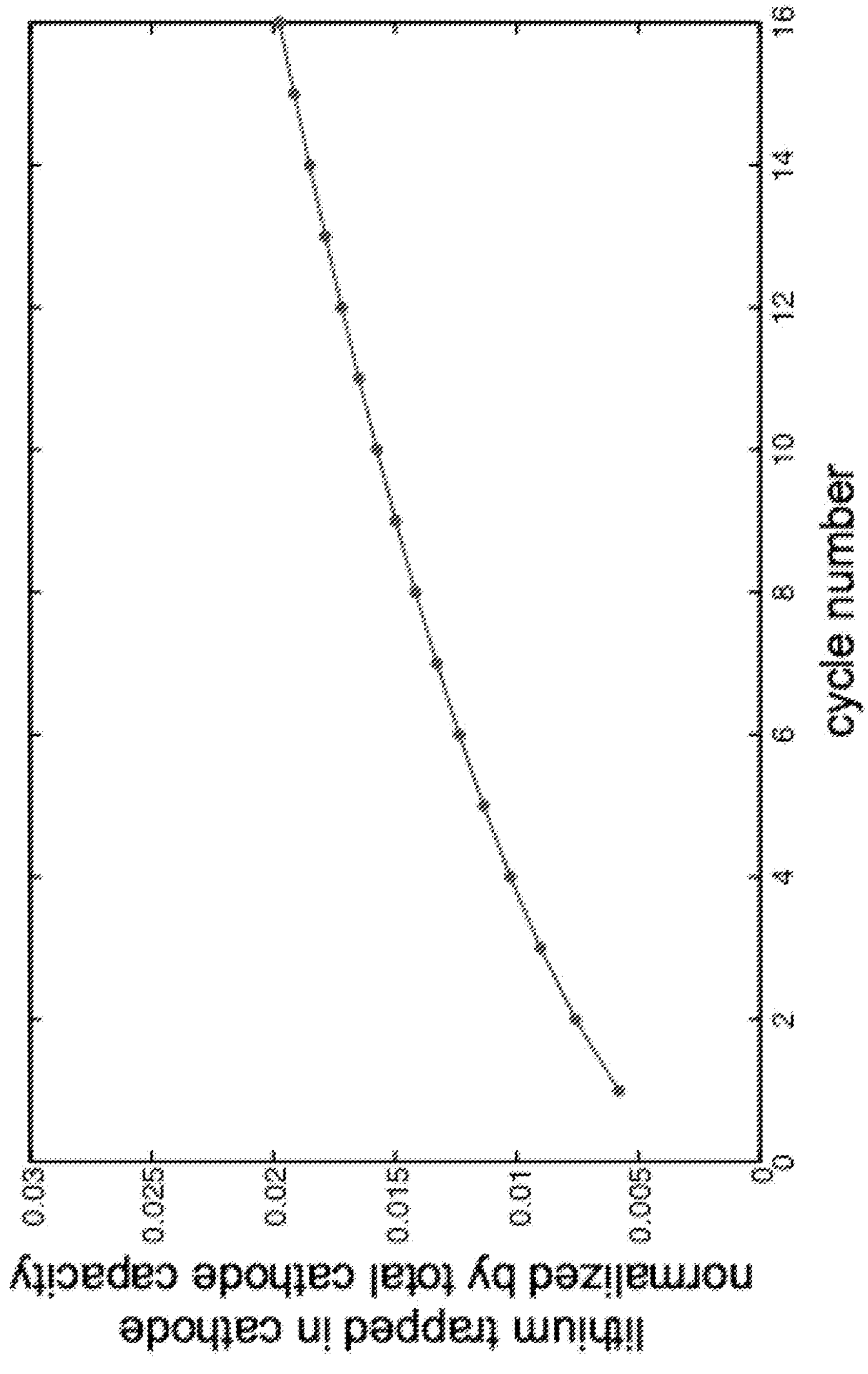

lithium trapped in cathode
normalized by total cathode capacity
0.03
0.025
0.02
0.015
0.01
0.005
0
0
2
4
6
8
10
12
14
16
cycle number

figure 20

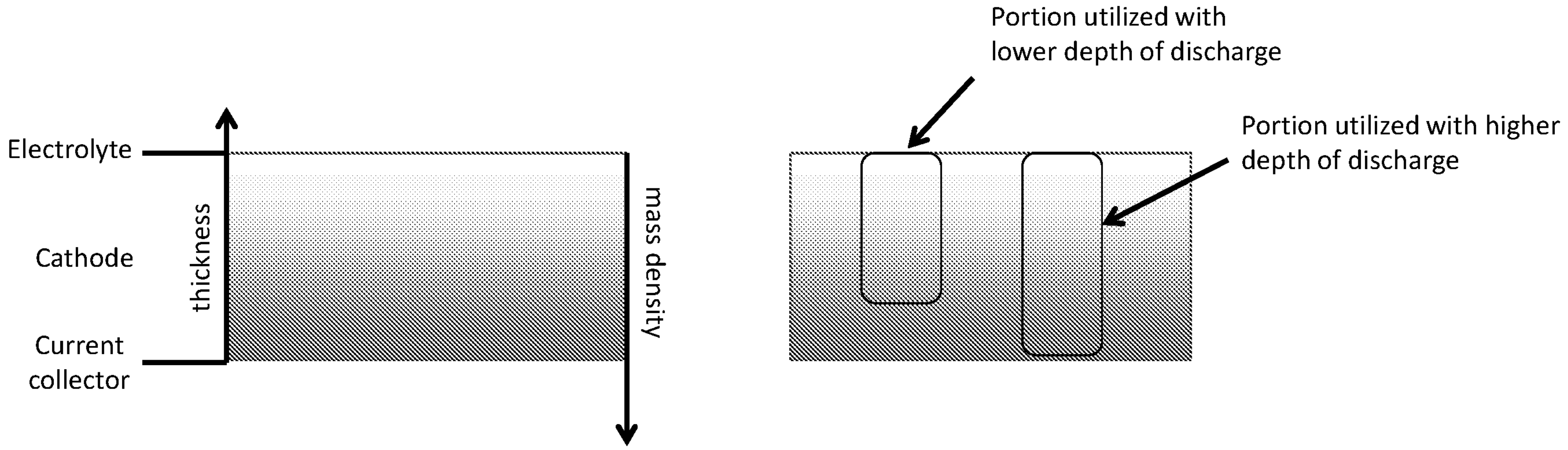
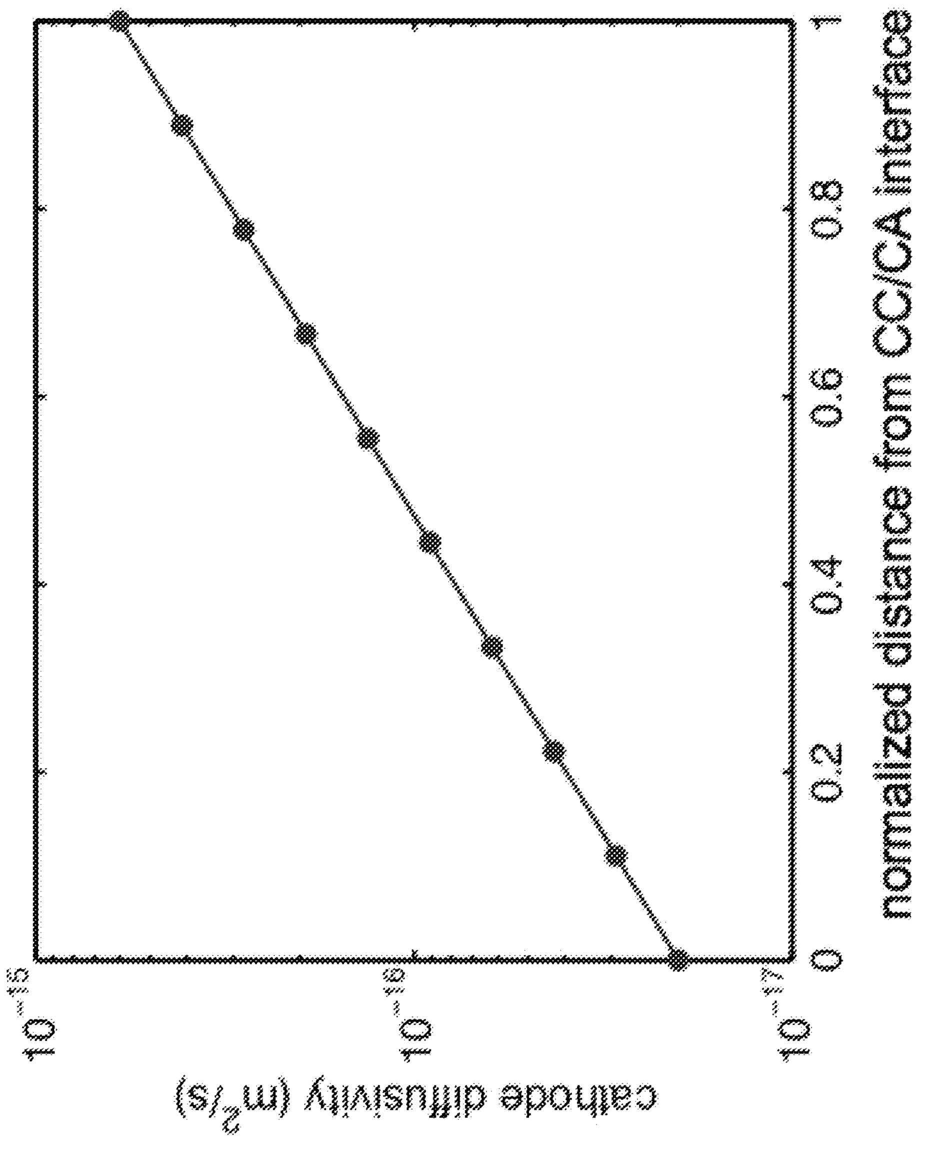

Electrolyte
Cathode
Current collector
thickness
mass density
Portion utilized with lower depth of discharge
Portion utilized with higher depth of discharge

figure 21



cathode diffusivity (m^2/s)
10^{-15}
10^{-16}
10^{-17}
0
0.2
0.4
0.6
0.8
1
normalized distance from CC/CA interface

figure 22A

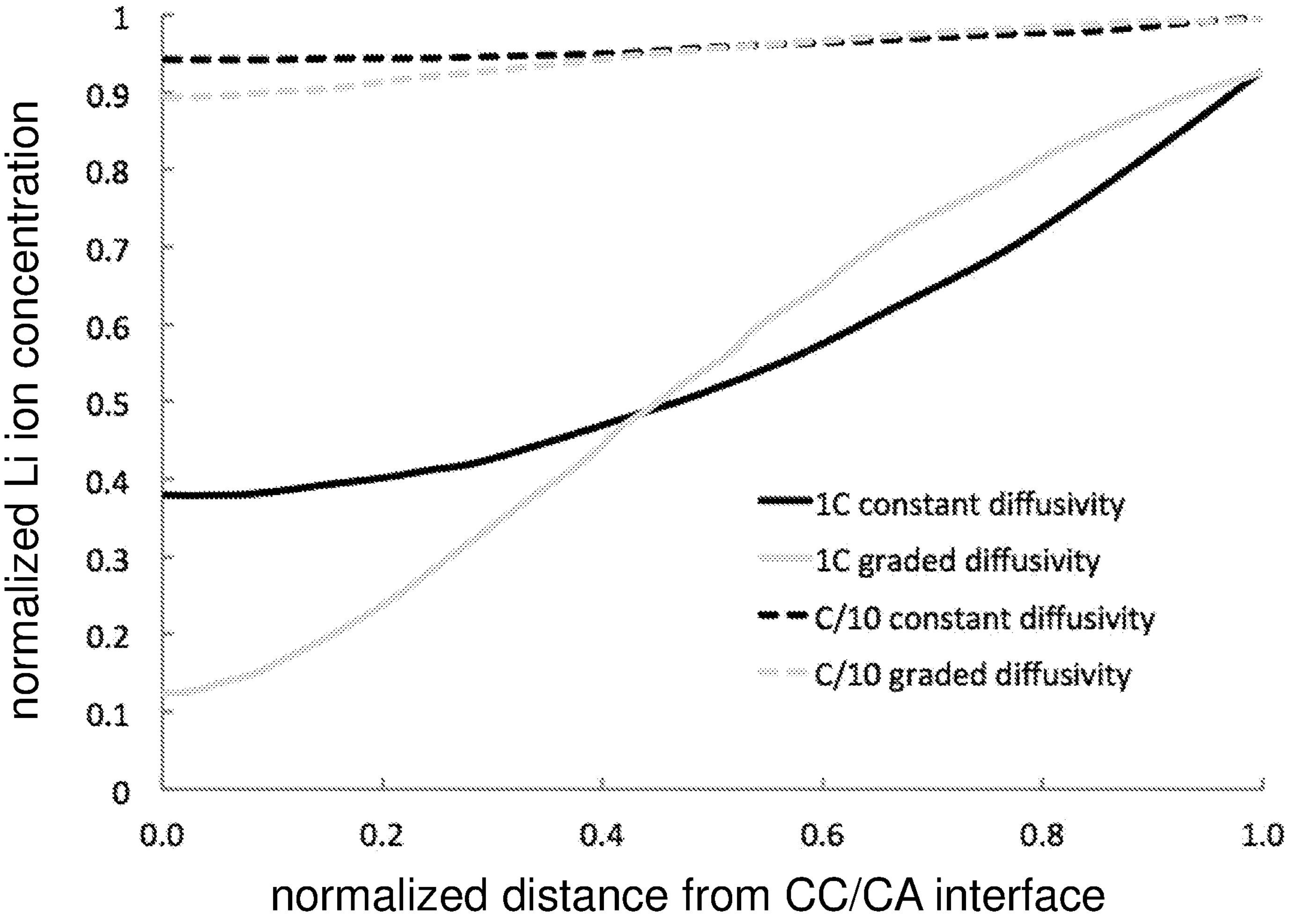

normalized Li ion concentration
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.0
0.2
0.4
0.6
0.8
1.0
normalized distance from CC/CA interface
1C constant diffusivity
1C graded diffusivity
C/10 constant diffusivity
C/10 graded diffusivity

figure 22B

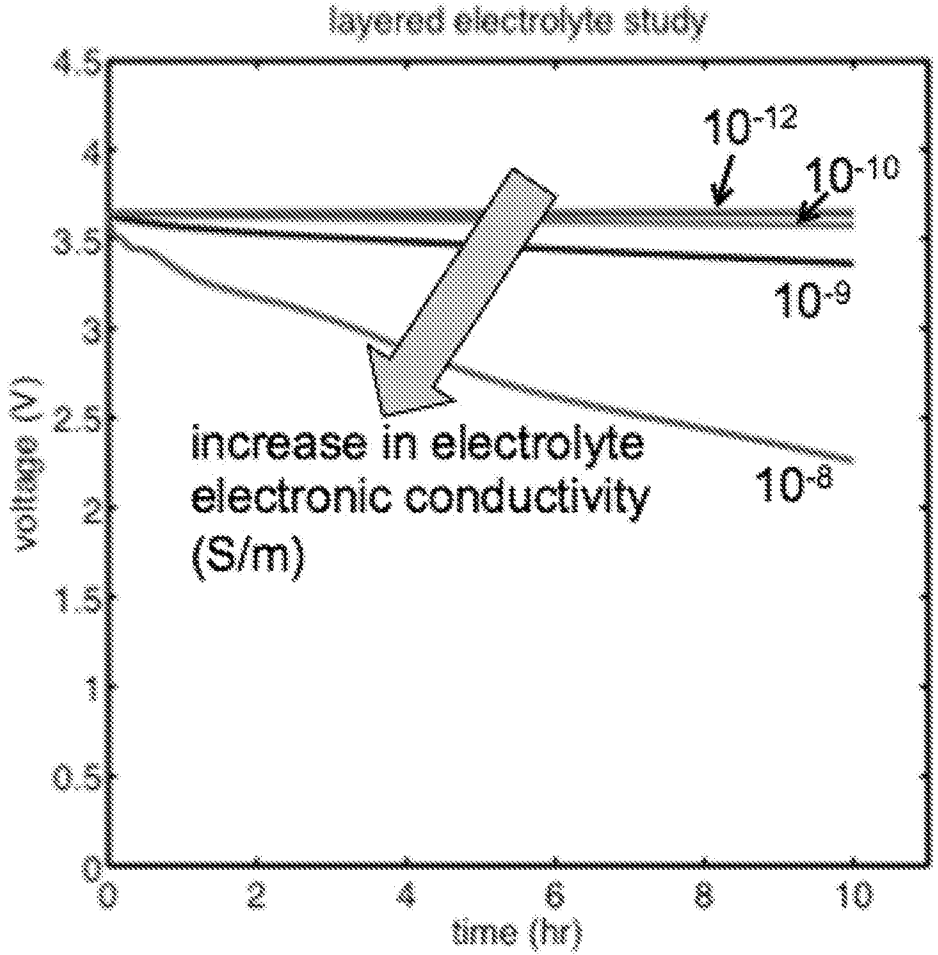

layered electrolyte study
voltage (V)
4.5
4
3.5
3
2.5
2
1.5
1
0.5
0
time (hr)
0
2
4
6
8
10
10-12
10-10
10-9
10-8
increase in electrolyte electronic conductivity (S/m)

figure 23

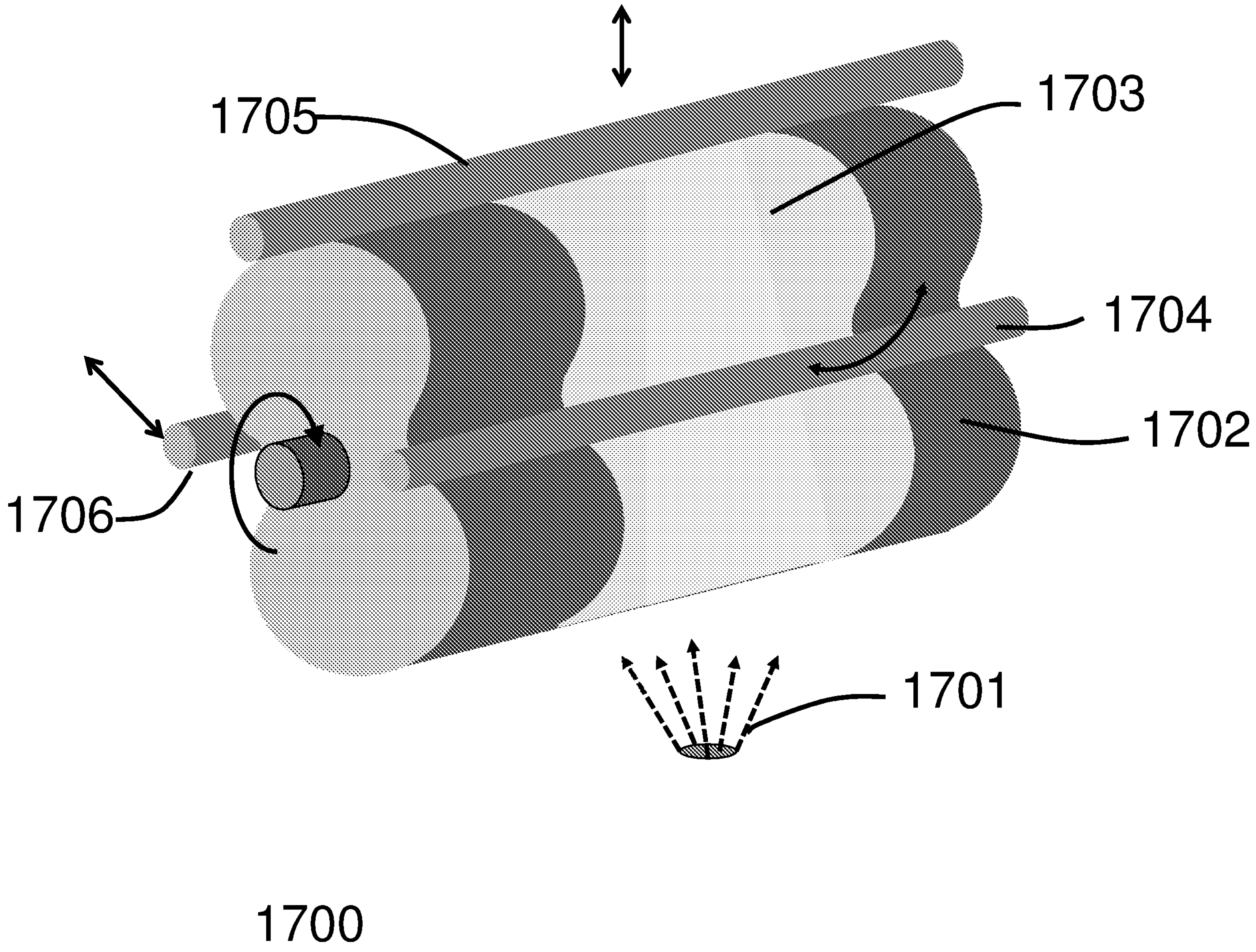


FIGURE 24

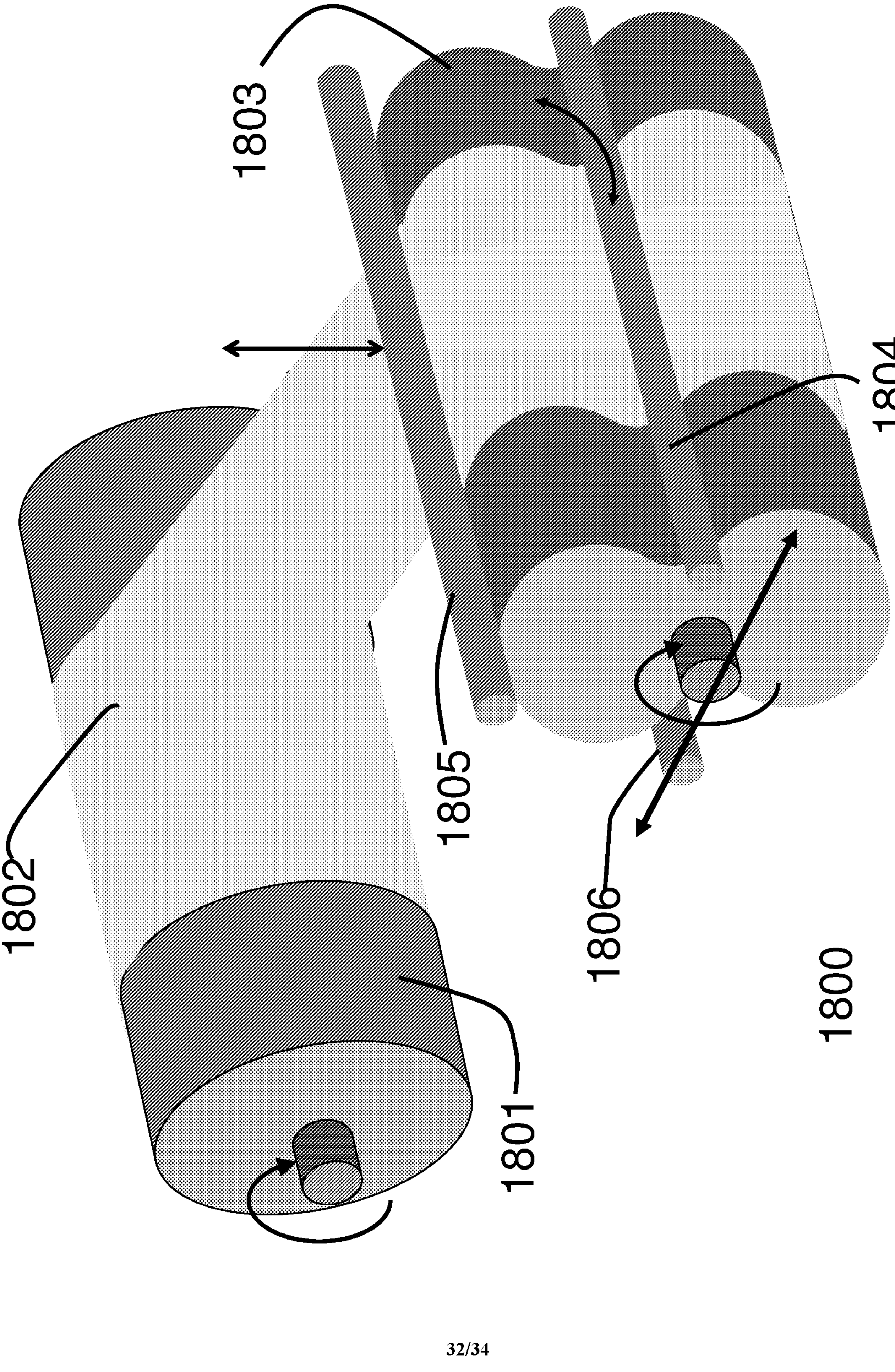


FIGURE 25

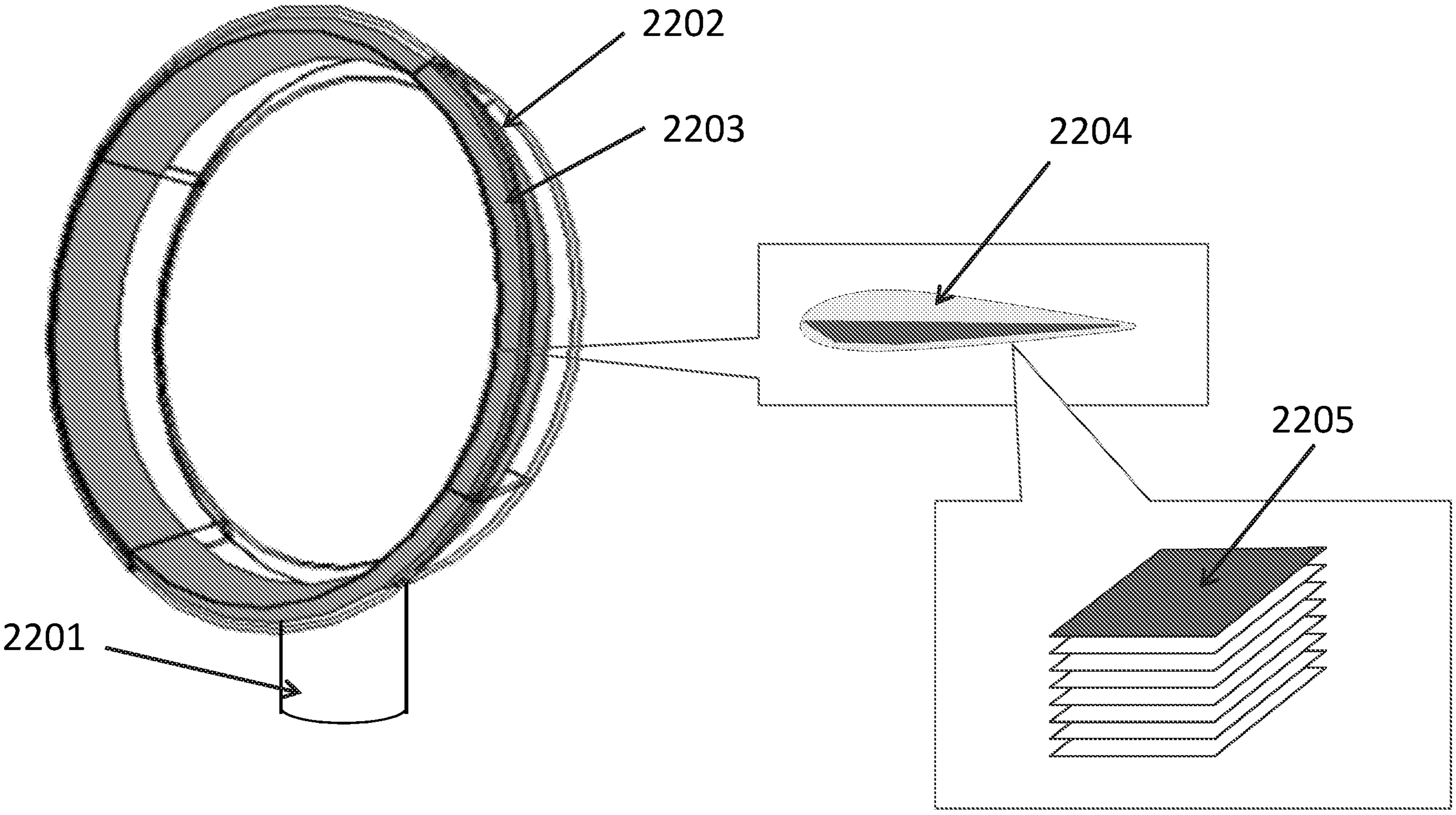


FIGURE 26A

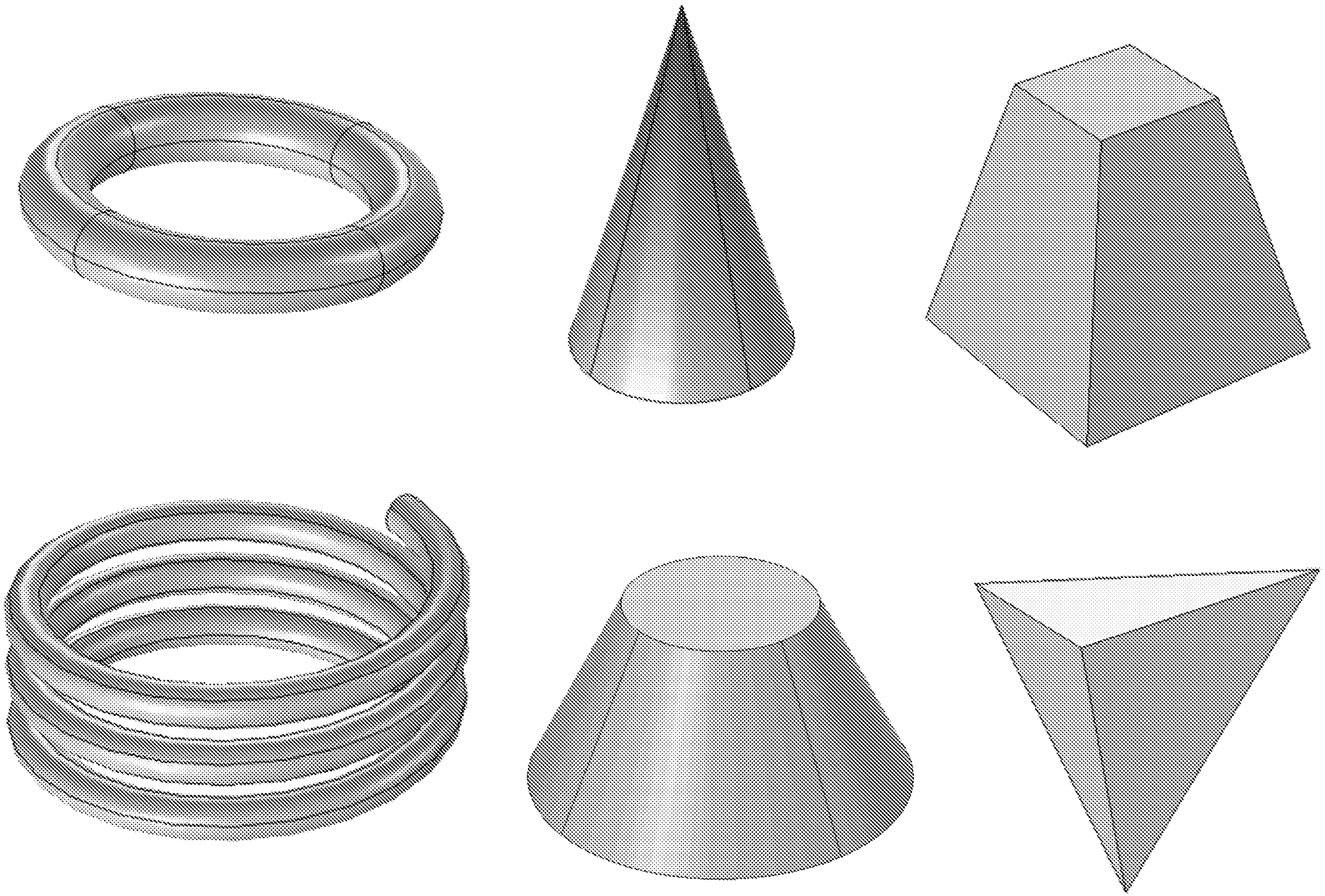


FIGURE 26B

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US15/66524

A. CLASSIFICATION OF SUBJECT MATTER

IPC(8) - H01M 4/13, 10/04; G06F 17/50 (2016.01)
CPC - H01M 4/139, 10/0565
According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)
IPC(8) Classifications: H01M 4/13, 10/04; G06F 17/30, 17/50, 19/00 (2016.01)
CPC Classifications: H01M 4/0423, 4/139, 10/0565; G06F 17/30, 19/00; Y02P 70/54; Y02E 60/122

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)
PatSeer (US, EP, WO, JP, DE, GB, CN, FR, KR, ES, AU, IN, CA, INPADOC Data, RU, AT, CH, TH, BR, PH); Google Scholar; EBSCO; IEEE; KEYWORDS: Computer aid design non aqueous layer solid state battery energy power density polymer film electrochemical cell three dimension lithium-ion process manufacture multilayer dielectric sheet contact resistance thermal expansion

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	US 2011/0202159 A1 (WANG, C et al.) August 18, 2011; figures 1, 3, 6a-6c, 8a; paragraphs [0009]- [0011], [0014]-[0015], [0036], [0038]-[0040], [0042], [0045]	1, 4, 11-15, 36, 39, 46-50, 52-55
Y		2-3, 5-10, 16, 37-38, 40-45, 51
Y	US 2012/0058380 A1 (WANG, C et al.) March 8, 2012; figures 3, 5; paragraphs [0009], [0040]-[0041], [0044], [0049]-[0050], [0056]	2-3, 16, 37-38, 51
Y	US 6,524,720 B1 (SHAH, G) February 25, 2003; column 6, line 36 to column 7, line 20; column 16, lines 44-55	5 & 40
Y	US 2009/0159451 A1 (TOMANTSCHGER, K et al.) June 25, 2009; paragraphs [0006] & [0114]	6 & 41
Y	US 5,672,214 A (ARTHUR, J et al.) September 30, 1997; column 6, lines 19-37; column 12, lines 41-67	7 & 42
Y	US 2012/0123401 A1 (SLATKINE, M) May 17, 2012; paragraphs [0047], [0064]-[0065], [0198], [0362]	8 & 43
Y	WO 2013/043203 A2 (THERANOS INC.) March 28, 2013; paragraph [0836]	9 & 44
Y	US 6,400,123 B1 (BEAN, H et al.) June 4, 2002; column 2, lines 18-33; column 7, lines 15-25; column 9, lines 38-59	10 & 45
A	US 2012/0046776 A1 (ZHANG, X et al.) February 23, 2012; entire document	1-16, 36-55

☐ Further documents are listed in the continuation of Box C. ☐ See patent family annex.

* Special categories of cited documents:
"A" document defining the general state of the art which is not considered to be of particular relevance
"E" earlier application or patent but published on or after the international filing date
"L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
"O" document referring to an oral disclosure, use, exhibition or other means
"P" document published prior to the international filing date but later than the priority date claimed
"T" later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
"X" document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
"Y" document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
"&" document member of the same patent family

Date of the actual completion of the international search 31 March 2016 (31.03.2016)	Date of mailing of the international search report 22 APR 2016
Name and mailing address of the ISA/ Mail Stop PCT, Attn: ISA/US, Commissioner for Patents P.O. Box 1450, Alexandria, Virginia 22313-1450 Facsimile No. 571-273-8300	Authorized officer Shane Thomas PCT Helpdesk: 571-272-4300 PCT OSP: 571-272-7774

INTERNATIONAL SEARCH REPORT

International application No.
PCT/US15/66524

Box No. II Observations where certain claims were found unsearchable (Continuation of item 2 of first sheet)

This international search report has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:

1. ☐ Claims Nos.:
because they relate to subject matter not required to be searched by this Authority, namely:

2. ☐ Claims Nos.:
because they relate to parts of the international application that do not comply with the prescribed requirements to such an extent that no meaningful international search can be carried out, specifically:

3. ☐ Claims Nos.:
because they are dependent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).

Box No. III Observations where unity of invention is lacking (Continuation of item 3 of first sheet)

This International Searching Authority found multiple inventions in this international application, as follows:
see extra sheet

1. ☐ As all required additional search fees were timely paid by the applicant, this international search report covers all searchable claims.

2. ☐ As all searchable claims could be searched without effort justifying additional fees, this Authority did not invite payment of additional fees.

3. ☐ As only some of the required additional search fees were timely paid by the applicant, this international search report covers only those claims for which fees were paid, specifically claims Nos.:

4. ☒ No required additional search fees were timely paid by the applicant. Consequently, this international search report is restricted to the invention first mentioned in the claims; it is covered by claims Nos.:
Claims 1-16 & 36-55

Remark on Protest
☐ The additional search fees were accompanied by the applicant's protest and, where applicable, the payment of a protest fee.
☐ The additional search fees were accompanied by the applicant's protest but the applicable protest fee was not paid within the time limit specified in the invitation.
☐ No protest accompanied the payment of additional search fees.

-***-Continued from Box III: Observations where unity of invention is lacking-***-

This application contains the following inventions or groups of inventions which are not so linked as to form a single general inventive concept under PCT Rule 13.1. In order for all inventions to be examined, the appropriate additional examination fee must be paid.

Group I: Claims 1-16 & 36-55 appear to be directed towards using one or more first or second characteristics to design a three dimensional multi-layered solid-state battery device.

Group II: Claims 17-35 appear to be directed towards using a numerical method to process one or more relationships, the one or more relationships being one or more coupled or decoupled, continuous, discretized, or piecewise continuous, partial or whole differential equations or other logical forms and using one or more first or second characteristics for a second three dimensional electrochemical device.

Group III: Claims 56-72 appear to be directed towards generating spatial information each layer geometry; storing the spatial information including each layer geometry into a database structure; selecting one or more material properties from a plurality of materials; using the one or more material properties with the spatial information in a simulation program; and outputting one or more performance parameters from the simulation program.

The inventions listed as Groups I-III do not relate to a single general inventive concept under PCT Rule 13.1 because, under PCT Rule 13.2, they lack the same or corresponding special technical features.

The special technical features of Group I are at least providing computer generated relationship between one or more first characteristics referenced against one or more second characteristics for a selected material set for design of three dimensional spatial elements in a three-dimensional electrochemical cell, selecting one or more of the first or second characteristics for the selected material set, and using the one or more first or second characteristics to design the three dimensional multi-layered solid-state battery device, which Groups II & III do not have. Group II has at least using a numerical method to process one or more relationships, the one or more relationships being one or more coupled or decoupled, continuous, discretized, or piecewise continuous, partial or whole differential equations or other logical forms, determining one or more first or second characteristics in a first three-dimensional electrochemical cell, and using the one or more first or second characteristics for a second three dimensional electrochemical device, which Groups I & III do not have. Group III has at least generating spatial information each layer geometry; storing the spatial information including each layer geometry into a database structure; selecting one or more material properties from a plurality of materials; using the one or more material properties with the spatial information in a simulation program; and outputting one or more performance parameters from the simulation program, which Groups I & II do not have.

The common technical features are at least a multi-layered solid-state battery device, one or more computer readable memory comprising: one or more computer codes for outputting a computer generated relationship between one or more first characteristics referenced against one or more second characteristics for a design of three dimensional spatial elements in a three- dimensional electrochemical cell, processing the one or more selected first or second characteristics to determine whether the one or more first or second characteristics is within predetermined performance parameters. These common technical features are previously disclosed by US 2012/0046776 A1 to Zhang, X et al. (hereinafter 'Zhang'). Zhang discloses a multi-layered solid-state battery device (a multi-layered solid state battery; paragraph [0033]), one or more computer readable memory comprising: one or more computer codes for outputting a computer generated relationship between one or more first characteristics referenced against one or more second characteristics for a design of three dimensional spatial elements in a three- dimensional electrochemical cell (a computer aided method comprising a memory and computer readable code for outputting a computer generated relationship between a first characteristic referenced against a second characteristic, via optimization, for design of three dimensional features of electrochemical cell unit layers; paragraph [0033], claims 7 and 15 of Zhang), processing the one or more selected first or second characteristics to determine whether the one or more first or second characteristics is within predetermined performance parameters (processing the second characteristic to determine if its within target requirements via optimization; paragraph [0033]).

Since these common technical features are previously disclosed by Zhang, they are not special and so Groups I-III lack unity.