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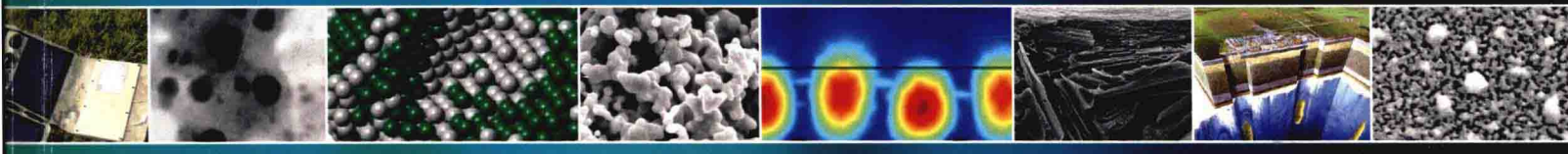
Materials for Energy, Efficiency and Sustainability



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MATERIALS FOR ENERGY, EFFICIENCY AND SUSTAINABILITY

Edited by
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PREFACE

TechConnect provides a multi-disciplinary and multi-sector forum focused on accelerating applied research and early-stage innovation towards commercialization. The technologies described in the TechConnect Briefs are provided by innovators working in industry, academic and government laboratories around the world. A review committee comprising more than 300 internationally recognized experts reviewed the research and innovations described and selected them for inclusion in this volume, and for presentation at the 10th annual TechConnect World Innovation Conference & Expo, held jointly with the 18th annual Nanotech Conference & Expo, and the 2015 National SBIR/STTR Conference, June 14-17, 2015 Washington DC.

Through TechConnect prospecting programs, transformational innovations are identified in Advanced Materials, Advanced Manufacturing, Materials for Energy & Sustainability, Electronics & Microsystems, Biotech, Medical & Pharma, Personal & Home Care, Cosmetics, and Food industries. The 2015 TechConnect Briefs are also aligned with the National Nanotechnology Initiative and the National Security Technology Accelerator interest areas.

This volume (one of 4) is focused on research and innovations in the Materials for Energy, Efficiency and Sustainability track, including industrially viable new materials that will transform industry and new platform technologies that enable their discovery and development. The following chapters are included:

- Energy Storage
- Fuel Cells & Hydrogen
- Nanomaterials for Catalysis
- Materials for Oil, Gas & Biofuels
- Carbon Capture & Utilization
- Solar Power Technologies
- Materials for Green Building
- Water Technologies
- Materials for Sustainability & Efficiency

It is our distinct honor to edit the 18th annual TechConnect publication of applied research technologies at the forefront of innovation change for industry and society. The TechConnect Program Committees make every effort to provide a scientifically and commercially relevant publication. The grassroots review and ranking process is a source of pride for these joint committees, and provides a yearly evaluation and technical validation of emerging technologies addressing our world's most pressing needs. We would like to take this opportunity to thank the many individuals who have worked so hard to make this annual publication possible. We hope that you enjoy these TechConnect Briefs, and we hope that the presented technologies are significant steps towards addressing large global challenges.

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Inclusion of Electromagnetic Stress to explain Lithiated Silicon Nanowires

Donald C Boone*

***-Nanoscience Research Institute - College Park, Maryland**

Abstract: This study considers the electromagnetic stresses and simulates the lithium insertion into a silicon nanowire. The resulting model uses a multi-physics approach to explain the two detrimental effects that could result during the lithiated silicon process: (1) The partial lithiation effects that are observed in some silicon nanowires under negligible volume expansion; (2) The excessive volume expansion that is observed after full lithium insertion with a resulting Cassini oval shaped silicon nanowire. Magnetic and electric fields are included in this computational model in order to introduce additional tensile and compressive stresses and as a result alters the band structure of the silicon nanowire as it transition from crystalline silicon (c-Si) structure to an amorphous lithiated silicon (a-LiSi) heterogeneous material.

1. The Continuum Model

The computational model that will be presented is based on the elastic-diffusion model of a silicon spherical nanoparticle that was presented in Golmon et-al. [1]. This model described the lithiation process from an electrochemical point of view. Lithium ions diffused through the crystalline silicon (c-Si) lattice, breaking silicon-silicon bonds and reforming lithium-silicon bonds, creating tensile stress throughout the nanoparticle while simultaneously Li-Si alloy material concentration builds up a compressive stress uniformly within the nanoparticle shell. Although the elastic-diffusion model does explain the volume expansion, it fails to explain for the slowing of the interfacial reaction front which is the interface between the c-Si and a-LiSi alloy that causes partial lithiation within the Si nanowire as was reported by Liu et-al. [2]. Therefore, an extension of this model is performed on a cylindrical silicon nanowire with the addition of electromagnetic theory. In the computational model or simulation that was performed, a series of partial differential equations (PDE) and trail functional (TF) were utilized to determine the effects of four solutions that comprised the varies stresses within our silicon nanowire model. The solutions of PDE with the use of TF are: 1) Elastic Displacement **u**, 2) Concentration $\overline{c}$, 3) Magnetic Field **B,** and 4) Electric Field **E** which culminates in radial stress equation

$$\sigma_r = \bar{E}\left[\frac{v}{2}\left(\frac{u}{R_c}\right) - \frac{\Omega}{6}\bar{c}\,(1+v) + \frac{aB}{\rho P}(1-2v)\right] \quad (1)$$

$$\text{where} \quad P = \epsilon_0 \chi E \quad (2)$$

where $\bar{E}$ is the modulus of elasticity, (v) is the Poisson constant, (a) is the lattice constant and R_c is the radius of curvature.

2. The Quantum Mechanical Model

Unlike continuum mechanics to describe the lithiation process in terms of varies stresses where a computer generated model was created from a large group of differential equations, the quantum mechanics approach that will be presented will use a heuristic method in examining the lithiated silicon process. Prior to the beginning of the lithiation process, there is no electron flow through the silicon nanowire. We will start the description of our model from the quantum mechanical perspective by developing the band structure of our pre-lithiated silicon nanowire. Silicon, which is a semiconductor material, is made up of band structures composed of valence and conduction bands which are separated by indirect band gap energy E_g. Silicon is a diamond cubic crystalline structure made up of tetrahedral molecules with its hybridized sp^3 orbitals within their valence shells filled with covalent bonding electrons from neighboring silicon atoms. Because the valence orbitals are completely filled, electron are not able to move freely within the crystal until a voltage is applied to the band structure. For silicon material, electrons within the valence band needs a minimum band gap energy of 1.1 electron volts in order to transition by way of trans-versing the band gap from the valence band to conduction band to create current flow. The Schrödinger equation is used to calculate the band structure by solving this eigenvalue equation in order to derive the band energies and wavefunctions of the individual electrons. For our model, we will use the Time-Dependent Schrödinger equation:

$$ih\frac{\partial \Psi}{\partial t} = H\Psi \quad (3)$$

The Hamiltonian is defined as

$$H = H_o + H_p \quad (4)$$

The total Hamilton (H) is composed of an initial or unperturbed Hamiltonian H_o that represents the state of the silicon nanowire before the start of lithiation and a perturbed Hamiltonian H_p that define the additional energy the nanowire will be subjected to by electromagnetic field. The unperturbed Hamiltonian H_o is defined as:

$$H_o = \frac{\bar{h}^2}{2m}\nabla^2 + V(r) + \frac{\bar{h}}{4m^2c^2}\frac{1}{\hat{R}} \cdot \nabla V \hat{S} \cdot \hat{L} \quad (5)$$

where $\hat{S}$ and $\hat{L}$ are defined as the spin and angular momentum operators respectively. The spin operator $\hat{S}$ are the Pauli matrices that are commonly used in quantum mechanics. The mass (m) is defined as the rest mass of the electron, h-bar $(\bar{h})$ is the Planck's constant, **c** the velocity of light and $\hat{R}$ is the position operator. The potential V(r) is a sum of several terms that are the interactions of the constitutive particles of this nanowire model namely silicon, lithium and electrons. The overall electric potential is defined as:

$$V(r) = V_{e-e} + V_{e-Si} + V_{e-Li} + V_{Si-Si} + V_{Si-Li} + V_{Li-Li} \quad (6)$$

The unperturbed Hamiltonian H_o is used in the **k·p** theory which is a mathematical method used to calculate the band structure in semiconductor materials such as silicon. In equation 5, the first term is the kinetic energy term (the **k·p** method formulates this term as being positive instead of negative as is the case in most Hamiltonians in Schrödinger equation), the second term as was mention is V(r) and the third term is the spin-orbital interaction term responsible for the energy that is generated from the interaction between the particles spin and orbital angular momentum. Figure 1 illustrates the conduction band structure due to H_o prior to the application of the electromagnetic fields at the moment lithium insertion begins. The band structure is crystalline silicon (c-Si) with an indirect band gap energy which are represented by the dispersion relation equations that are the result of the solution of the Schrödinger equation using the unperturbed Hamiltonian H_o.

Minimum conduction band

$$E_c = E_{k0} + \frac{\bar{h}^2k^2}{2m} + \frac{\bar{h}^2}{E_{Si}m^2}\sum_n |\langle u_c|\mathbf{k}\cdot\mathbf{p}|u_v\rangle|^2 \quad (7)$$

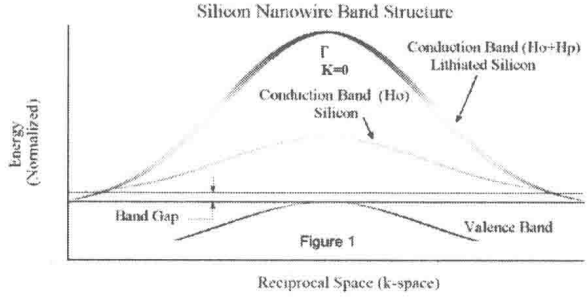
and the maximum valence band

$$E_v = -\frac{\bar{h}^2k^2}{2m} \quad (8)$$

where $E_{k0} = E_{k0}(0,t)$ is an energy coefficient, **k** is the wavevector, $\hat{p}$ the momentum operator, u_c and u_v are gaussian functions for the conduction and valence bands respectively, and E_{Si} is the band gap energy of silicon. This as was stated previously is a constant at 1.1 eV. From equations 7 the effective mass m_{eff} can be derived as

$$\frac{1}{m_{eff}} = \frac{1}{m} + \frac{2}{E_g m^2}\sum_n |\langle u_c|\mathbf{k}\cdot\mathbf{p}|u_v\rangle|^2 \quad (9)$$

and E_g is in general the band gap energy.



The perturbed Hamiltonian H_p is the energy added to the silicon nanowire the moment lithiation process begins. H_p is defined as:

$$H_p = -\frac{e}{2\,m_{eff}c}\mathbf{B}\cdot\hat{\mathbf{L}} + \frac{e^2}{8\,m_{eff}c}[\mathbf{B}^2\mathbf{r}^2 - (\mathbf{B}\cdot\mathbf{r})^2] + \frac{e^2E^2}{2\,m_{eff}\omega^2} \quad (10)$$

where (e) is the electron charge and (ω) is the angular frequency of the electric field. In our computational continuum model, the applied electric field **E** and magnetic field **B** magnitudes are of a small scale to a degree that the electric field **E** is just above the threshold to allow electrons from the silicon to transition from valence band to the conduction band. The magnitude of the applied magnetic field **B** is several orders below the electric field **E**. When the lithiation process begins, this initiates a process of transforming from crystalline silicon (c-Si) to an