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Maxwell stress to explain the mechanism for the anisotropic expansion in lithiated silicon nanowires

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This computational research study attempts to explain the process that leads to volume expansion during insertion of lithium ions into a silicon nanowire. During lithiation, electrons flow through the nanowire in the opposing direction of lithium ions insertion. This causes an applied electromagnetic field which is described as being a quantum mechanical version of photon density wave theory. A series of events are calculated as the individual electrons and photons travels through the lithiated silicon nanowire. The hypothesis that will be presented employs the Maxwell stress tensor to calculate the refractive indices in three orthogonal directions during lithiation. The quantum harmonic oscillator and the electromagnetic intensity will be utilized in this presentation to calculate the energy of electrons and optical amplification of the electromagnetic field respectively. The main focus of this research study will use electron scattering theory, spontaneous and stimulated emission theory to model the breaking of cohesion bonds between silicon atoms that ultimately leads to excessive volume expansion that is witnessed during the lithiation process in Si nanowires. © 2016 Author(s). All article content, except where otherwise noted, is licensed under a Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/).

I. INTRODUCTION

The current research body of knowledge for lithiated silicon anode materials has been exclusively focused on lithium ion diffusion process. The research work by Liu et al., anisotropic volume expansion of lithiated silicon nanowires was studied employing transmission electron microscope (TEM) and electron diffraction pattern (EDP). The measured results were that crystalline Li$_x$Si, at $x = 3.75$ formed immediately upon full lithiation. The morphology evolution of the lithiated silicon nanowire started from a pristine crystalline silicon (c-Si) nanowire at 155 nm in diameter prior to lithium insertion to 17% diameter increase in the $<111>$ direction while a 170% increase in diameter of 485 nm was measured in the $<110>$ direction after full lithiation. In addition, a crack along the longitudinal direction of $<112>$ was detected. This gave the expanded lithiated silicon nanowire a described “dumbbell cross section” shape that resembled Cassini oval curve geometry.

The research study performed by Cubuk et. al. used kinetic Monte Carlo (kMC) method to simulate the different expansion rates of the interfacial reaction fronts within the silicon nanowire during lithium insertion. This research study confirms the experimental findings that was stated previously where the lithium ion insertion was 7 times faster in the $<110>$ direction than the $<111>$ direction. The work drawn from Jung et. al. MD/DFT simulation was created to study the atomistic behavior at the crystalline silicon-amorphous lithiated silicon interfacial reaction front. A common minimum interfacial energy was discovered in lithiated silicon (Li$_x$Si) where $x = 3.4$ which closely mirrors the TEM work of Liu et.al. where $x = 3.75$ is the composite ratio of crystalline lithiated silicon.

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II. MATHEMATICAL FRAMEWORK

The computational model that is chosen for our research study is a quantum harmonic oscillator that is encased within a single silicon diamond lattice (Figure 1). The software that will be utilized for the computational model of our study will be MATLAB® version R2013a mathematical software. The data from MATLAB will be exported to Microsoft EXCEL 2013 in order to create charts that will be presented near the end of this study. Our presentation is based on first principles well established theories in various disciplines within physics especially quantum mechanics. Therefore, we will start with the Schrödinger equation which is used to calculate the band structure by solving this eigenvalue equation in order to derive the band energies and wave functions of the individual electrons. For our model, we will use the time-independent Schrödinger equation:

\[ H \Psi = E \Psi \]  

where the Hamiltonian (H) is defined as

\[ H = H_o + H_p \]  

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 the applied electromagnetic field. The unperturbed Hamiltonian H_o is defined as:

\[ H_o = -\frac{\hbar^2}{2m} \nabla^2 + V(r) + \frac{1}{4m^2c^2} \sum \frac{1}{\hat{R}} \nabla V \hat{S} \cdot \hat{L} \]  

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, \( \hbar \) is the Planck’s constant, c the velocity of light and \( \hat{R} \) is the position operator. In Equation (3), the first term is the kinetic energy, the second term V(r) is the potential energy and the third term is the spin-orbital interaction responsible for the energy that is generated from the interaction between the electrons spin and orbital angular momentum. The use of the silicon wave function \( \psi_n(r, \theta, \phi) \) for each of the four core atoms located within the silicon lattice will be used as a starting point in our computations

\[ \psi_n(r, \theta, \phi) = N \alpha^{n-1} e^{\frac{Z_{eff}(\alpha, n)}{2m}} Y_l^m(\theta, \phi) \]  

FIG. 1. Silicon is a diamond crystalline cubic 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.
where \( r, \theta, \phi \) are the spherical coordinates, \( n \) the energy level, \( Z_{\text{eff}} \) is the effective atomic number, \( N \) is the normalization constant, \( a_o \) is Bohr radius and \( Y^m_l (\theta, \phi) \) is the spherical harmonics of the silicon atom. The silicon ground state wave function \( \Psi^{g}_{Si} \) is calculated using the Slater determinant
\[
\Psi^{g}_{Si} = \begin{bmatrix}
\psi_1(R_1S_1) & \psi_2(R_2S_2) \\
\psi_3(R_3S_3) & \psi_4(R_4S_4)
\end{bmatrix}.
\] (5)

The silicon ground state wave function \( \Psi^{g}_{Si} \) is composed of the four core silicon atoms within the lattice that will be used to model the silicon background and maximum valence band within the cubic lattice prior to the introduction of lithium ions and electron flux (Figure 1). With establishing the maximum valence band, in order to construct the minimum conduction band, a Bloch function based on electron scattering theory is used
\[
u_c(r) = e^{ikr} + \frac{1}{kr} e^{i(kr + \delta)} + \frac{3z}{kr} e^{i(kr + \delta)} \sin \delta
\] (6)
with position vectors \( r \) and \( z \), wavenumber \( k \) and phase shift \( \delta \) define as variables and functions within the equation. The Bloch function consist of three terms, the first term is known as the incident wave function and the second and third term collectively is called the scattering wave function. When an electron is traveling in the conduction band the first term of the wave function describes the electron from a point before impact with the oncoming atom (incident wave function) and the second and third term of the wave function describes the electron after impact with the colliding atom (scattering wave function). The current density \( J \) is calculated with the use of the Bloch function
\[
J = -\frac{ie\hbar \nu_{DOS}}{2m} \left( u_c \nabla u_c^* - u_c^* \nabla u_c \right)
\] (7)
where \( \nu_{DOS} \) is define as the density of state volume within our model. In order to simulate the flow of electrons through the silicon nanowire, the excited state wave function for lithium \( \Psi^m_{Li} \) is constructed by using time-independent perturbation theory
\[
\Psi^m_{Li} = \frac{(\Psi^m_{Li}|H_p|\Psi^g_{Li})}{(E_o - E^g_{Li})} \Psi^g_{Li}
\] (8)

The orthogonal wavefunction is \( \Psi^m_{Li} \) and \( E_o \) and \( E^g_{Li} \) are the ground state energies for \( \Psi^g_{Li} \) and \( \Psi^m_{Li} \) respectively. The perturbed Hamiltonian \( H_p \) simulate the electromagnetic energy added to the silicon nanowire the moment lithiation process begins. \( H_p \) is defined as:
\[
H_p = -\frac{e}{2m_{\text{eff}}} \mathbf{B} \cdot \mathbf{L} + \frac{e^2}{8m_{\text{eff}}} \left( B^2r^2 - (B \cdot r)^2 \right) + \frac{e^2E^2}{2m_{\text{eff}}\omega^2} \] (9)
where \( e \) is the electric charge of an electron, \( m_{\text{eff}} \) is the electron effective mass and \( \omega \) is the angular momentum of the electron as it travels in the conduction band. The applied electric field \( \vec{E}_{ij} \) and magnetic field \( \vec{B}_{ij} \) are defined as
\[
\vec{E}_{ij} = iC_{Eij} \frac{\hbar}{4n_{c}e} \left[ u_c \nabla u_c^* - u_c^* \nabla u_c \right] e^{2\gamma_{ij}}
\] (10)
\[
\vec{B}_{ij} = iC_{Bij} \frac{\hbar}{2n_{c}e} \left[ u_c \nabla u_c^* - u_c^* \nabla u_c \right] e^{2\gamma_{ij}}
\] (11)
where \( n_c \) is defined as the net charge within the quantum harmonic oscillator conduction bands per unit volume, \( n_c \) is the electron density of the maximum valence band and \( \gamma_{ij} \) is the optical amplification that will be explained later in is study. The coefficients \( C_{Eij} \) and \( C_{Bij} \) are for the electric and magnetic fields that will allow these fields to be a solution to Maxwell equations. The energy density \( \mathcal{E}_{ij} \) of the applied electromagnetic (EM) field is defined as
\[
\mathcal{E}_{ij} = \frac{1}{2} \left( \varepsilon_{ij} \vec{E}_{ij}^2 + \frac{1}{\mu_{ij}} \vec{B}_{ij}^2 \right)
\] (12)
with $i$ and $j$ are indices with values 1, 2 and 3, $\gamma_{ij} = \epsilon_o \gamma_{ij}$ is the relative electric permittivity which is the constitutive property that defines how the dielectric material affects an applied electric field and $\epsilon_o$ is the vacuum electric permittivity. The relative magnetic permeability $\mu_{ij}$ is the constitutive property that defines the amount of magnetization a material has in response to an applied magnetic field. The magnetization is the magnetic moments per unit volume which is in essence the magnetic property that defines the amount of magnetization a material has in response to an applied magnetic field. The magnetization is negligible which results in $\mu_{ij}$ being define as unity or one. Equation (12) is also known as the Maxwell stress tensor.\textsuperscript{12} When $i = j$, the three orthogonal directions that were discussed in the introduction, namely <110>, <111> and <112>, will be given the matrix element $\epsilon_{11}$, $\epsilon_{22}$ and $\epsilon_{33}$ respectively and are called the electric susceptibilities $\epsilon_{ij}$ for lithiated silicon. For each of these directions we will designate a matrix element on the principle diagonal of the dielectric tensor.\textsuperscript{13}

\[
\epsilon_{ij} = \begin{bmatrix} \epsilon_{11} & \epsilon_{12} & 0 \\ \epsilon_{21} & \epsilon_{22} & 0 \\ 0 & 0 & \epsilon_{33} \end{bmatrix}^{-1}
\]

\[
\epsilon_{11} = \frac{\omega_o^2 X_{11}}{\omega_{11}^2 - \omega_o^2} \quad \epsilon_{22} = \frac{\omega_o^2 X_{22}}{\omega_{22}^2 - \omega_o^2} \quad \epsilon_{33} = \frac{\omega_o^2 X_{33}}{\omega_{33}^2 - \omega_o^2} \quad \epsilon_{12} = -\epsilon_{21} = \frac{\omega_o^2 X_{12}}{\omega_{12}^2 - \omega_o^2}
\]

\[
\omega_{yij} = \frac{a^3}{2\hbar} \left[ \gamma_{yij} \bar{E}_{ij}^2 + \frac{1}{\mu_{ij}} \bar{B}_{ij}^2 \right]
\]

\[
\omega_{nij} = \left[ \frac{4\pi \epsilon_o M_{ij} a^3 \bar{E}_{ij}^2}{Z_{Si} e m_{el}} \right]^{\frac{1}{2}}
\]

\[
\omega_p = \frac{1}{\hbar} \langle \Psi_{Li}^p | \vec{H}^* | \Psi_{Li}^p \rangle
\]

\[
\chi_{ij} = \frac{e^2 \rho \omega_f}{\hbar a^2} \left[ \langle \Psi_{Li}^e | \bar{r}_{ij} | \Psi_{Li}^e \rangle \right] \left[ \frac{1}{\omega_p - \omega_yij} + \frac{1}{\omega_p + \omega_yij} \right]
\]

where $\omega_p$ is the excited state energy per $\hbar$ experienced by the lithium ion when they are in excitation, $\omega_yij$ is the energy per $\hbar$ of the applied electromagnetic field, the silicon lattice cube volume of Figure 1 is defined by $a^3$, $\omega_{nij}$ is the resonant angular frequency of the silicon atoms. Analyzing the parameters of Equation (16), $M_{ij}$ is the elastic modulus tensor for silicon, $a_{Si}$ is the silicon atomic radius and $Z_{Si}$ the atomic number of silicon.\textsuperscript{14} The electric susceptibilities for lithium $\chi_{ij}$ is defined by the ground state lithium ion $\Psi_{Li}^e$ and excited state lithium ion $\Psi_{Li}^e$ wave functions, the resistivity $\rho$ of lithium ions within the silicon cubic lattice and the collision frequency $\omega_f$ of electrons define as the number of collisions per unit time an electron has between collisions with lithium-silicon particles.

III. COMPUTATIONAL MODEL

Prior to the beginning of the silicon nanowire lithiation process, the individual lithium atoms are ionized within the lithium metal electrochemical solid cell (W) reducing them to the constitutive particles of lithium ions and free electrons.\textsuperscript{15} The electrons and lithium ions will enter the silicon nanowire at opposing ends and therefore travel in opposite directions. Figure 2 displays the schematics of the silicon nanowire during lithium ion and electron flow insertion.

When the lithiation process begins, this initiates a process of transforming the silicon from crystalline silicon (c-Si) to an amorphous lithiated silicon (a-LiSi) molecules.\textsuperscript{16,17} A voltage of 2-V.
FIG. 2. In-situ experimental arrangement for a solid electrochemical cell using lithium metal counter electrode.

FIG. 3. Spontaneous Emission.

is applied to the apparatus in order for lithiation process to begin. The electron flux is not constant, in fact steadily increases with the continue diffusion of lithium ions within the silicon nanowire. Since the electrons are moving charge particles they are the source of the applied quantized electromagnetic field.

The applied electromagnetic field that are composed of photons splits the energy levels within the lithium ions due to applied electric field (Stark Effect) and by the applied magnetic field (Zeeman Effect). When photons are absorbed by a lithium ion, the ion experiences an excitation which transitions the lithium ion from the ground state to excited state. The electrons in the excited lithium ion transitions to a higher discrete energy level. Once the lithium ion transition to an elevated energy level it is subjected to the spontaneous emission process as displayed in Figure 3.

Lithium ions during the diffusion process increases the density ratio of lithium to silicon atoms define by $x$ in $\text{Li}_x\text{Si}$. The increase in $x$ signifies that the lithium ions are increasing in number within the silicon lattice. With the continuation of photons absorbing into the diffused lithium ions causing excitation and at the same time the diffusion process causes an increase in lithiated silicon density, the total atomic system in our lithiated silicon lattice model experiences population inversion which is define as a majority of atoms or ions being in the excited state. When the lithium ions are in such a state with photons being transmitted and absorbed within this dense lithium-silicon particle matrix, populated inversion is the prelude to stimulated emission process (Figure 4).

Stimulated emission occurs when an incoming photon interacts with a lithium ion in the excited state inducing it to transition an electron to the ground state emitting a photon that is approximately

FIG. 4. Stimulated Emission.
of the same frequency, phase and direction of the incoming photon. These photons, which are in the electromagnetic mode and are analogous to oscillating waves, are said to be in a state of coherence. The photons interfere with each other constructively instead of destructively. The start of stimulated emission with the majority of lithium ions in population inversion causes the electromagnetic intensity \( I \) to increase exponentially. The initial EM intensity \( (I_0) \) is define as
\[
I_0 = \frac{E \times B}{\mu_0 \hbar \omega c}
\]
which is a part of photon density wave theory.\(^{21}\) This exponential increase in \( I \) is define by a group of equation that includes Einstein coefficients that are used in spontaneous and stimulated absorption and emission rates:
\[
I(\mathbf{r}, t) = I_0 e^{\gamma_{ij}(r, t)}
\]
where
\[
\gamma_{ij}(r, t) = \sigma_{21ij} \cdot \Delta N_{21}
\]
\[
\Delta N_{21} = (N_2 - N_1)
\]
\[
\sigma_{21ij} = A_{21ij} \frac{\lambda^2}{8\pi n_j^2} g(\omega)
\]

\[\text{Maxwell Stress Tensor}\]

\[\text{Maxwell Stress Tensor}\]

**FIG. 5.** The above charts demonstrates photonic energy of the applied electromagnetic field for the \(<110>\), \(<111>\) and \(<112>\) orthogonal directions versus the negative charge differential. The oscillatory nature of the electromagnetic field energies is derived from the wavelike nature of the electric and magnetic fields.\(^{22}\)
\[ A_{21ij} = \frac{4e^2 \omega_p^3}{3\hbar c^3} \left| \left\langle \Psi_e^r | r | \Psi_e^l \right\rangle \right|^2 \left( \omega_p - \omega_{ij} \right) . \] (24)

In Equation (22), \( \Delta N_{21} \) is the difference of the number of excited state atoms \( N_2 \) and the number of ground state atoms \( N_1 \) within our model. For this study we select only the lithium ions to be in the excited state, \( N_2 = 30 \) and only the silicon atoms to be in the ground state \( N_1 = 8 \). Therefore, a ratio of \( x = N_2/N_1 \) equals 3.75 which is the same \( x \) in \( \text{Li}_x\text{Si} \) and at which the silicon diamond cubic lattice in our model is considered to be fully lithiated. Equation (23) is the stimulated emission cross section area \( \sigma_{21ij} \) which is define by Einstein A Coefficient \( A_{21ij} \), the spectral line shape function \( g(\omega) \), wavelength of the photon emitted \( \lambda \) and the refractive index \( n_{ij} \) of the electromagnetic field which is defined

\[ n_{ij} = \sqrt{\varepsilon_{ij} \mu_{ij}} \] (25)

where \( \mu_{ij} = 1 \). Collectively these equations describe the process called optical amplification. The electromagnetic field increases with the magnitude of \( e^{\frac{\gamma_{ij}r^2}{2}} \) as noted in Equations (10) and (11). As first mentioned in the electric and magnetic field equations, the variable \( n_c \) is define as the negative charge differential within the quantum harmonic oscillator conduction bands per unit volume which is the difference between the electrons that are traveling in the conduction bands and the number of positively charge lithium ions within silicon cubic lattice model. Theoretically, there is no applied electromagnetic field if there are an equal number of electrons and lithium ions within the model.\(^2\)

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**FIG. 6.** (a) The electric susceptibility \( \varepsilon_{ij} \) trends downwards in all three directions as \( n_c \) increases. (b) The electromagnetic intensity is much higher in the \(<110>\) direction than \(<111>\) and \(<112>\) which could be the reason for the faster rate of expansion in the \(<110>\) direction that were documented in TEM research study\(^1\) and DFT/MD simulations.\(^5\)
When the number of electrons are greater than the lithium ions an applied EM field is created. When the electrons enter the silicon nanowire, at first the electrons travel through c-Si before making contact with lithium ions. At this point the electric and magnetic fields are extremely weak. The electric field is of the order of $10^{-15}$ and the magnetic field $10^{-22}$. The energy that is stored in the applied electromagnetic field is of the magnitude of $10^{-44}$ eV. However, when electrons cross the interfacial reaction front that separates c-Si and Li$_x$Si the EM field increases by the order of $10^{23}$ due to the metallic properties of lithium.

At this point when electrons and lithium ions make contact and $n_e$ is non zero, the EM field diverges into the three orthogonal components of $\langle 110 \rangle$, $\langle 111 \rangle$ and $\langle 112 \rangle$ as mentioned earlier in this study (Figures 5(a) and 5(b)). The three electric fields are of the order of $10^9$. However, the magnetic field is of the order of $10^9$ and thus negligible contributions to the EM field.

When $n_e \approx 6$ in the $\langle 110 \rangle$ direction there is a great surge in the applied electromagnetic (EM) energy due to the Maxwell stress tensor. When the applied EM field stores this much energy the individual photons that comprises the quantized electromagnetic field are energetic enough to break covalent bonds between silicon atoms which are 9.26 eV.\textsuperscript{23} Similarly, in the other orthogonal directions of $\langle 111 \rangle$ and $\langle 112 \rangle$ there are surges of EM energy however at $n_e \approx 13$ and 19 respectively. The surges in energy in the EM field is cause by optical amplification which is due to stimulated emission. In addition, as the electromagnetic field increases the refractive indices $n_{ij}$ in all three orthogonal directions decreases which contributes to the overall amplification of the EM field and EM energy (Figures 6(a) and 6(b)).

IV. SUMMARY

It is the hypothesis of this author that to fully understand the electrochemical kinetics process of the lithiated silicon nanowire on the macroscopic level, quantum coherence states\textsuperscript{24} and photon density wave\textsuperscript{27,28} theories needs to be employed. The reaction rates between the orthogonal directions that were determine by Liu et al\textsuperscript{1} to be seven times greater in the $\langle 110 \rangle$ direction compared to the $\langle 111 \rangle$ can also be explained through these two treatments. This is not the focus of this work presented in this paper. However, what can be said about electrochemical kinetics in regards to this research is that the amplified EM field energy that is the result of stimulated emission process is analogous to the overpotential that is experience at the macroscopic level of electrochemical kinetics represented by the Butler-Volmer equation.\textsuperscript{26} For a conventional battery, mass transfer of electrons and ions that is represent in the exchange current density of the Butler-Volmer equation is used to transfer charged particles between the electrode and electrolyte whereupon a large potential difference or voltage accumulates on the electrode which induces energy. For the lithiated silicon nanowire instead of mass transfer process, the energy transfer process defines the electrochemical kinetics. Once the electrons passes through the interfacial reaction front they become energetic whereupon they augment the applied EM field by producing photons with energy great enough that could break silicon cohesion bonds.\textsuperscript{27,28}

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