Finite Element Analysis of Silicon Thin Films on Soft Substrates as Anodes for Lithium Ion Batteries

by

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ABSTRACT

The wide-scale use of green technologies such as electric vehicles has been slowed due to insufficient means of storing enough portable energy. Therefore it is critical that efficient storage mediums be developed in order to transform abundant renewable energy into an on-demand source of power.

Lithium (Li) ion batteries are seeing a stream of improvements as they are introduced into many consumer electronics, electric vehicles and aircraft, and medical devices. Li-ion batteries are well suited for portable applications because of their high energy-to-weight ratios, high energy densities, and reasonable life cycles. Current research into Li-ion batteries is focused on enhancing its energy density, and by changing the electrode materials, greater energy capacities can be realized. Silicon (Si) is a very attractive option because it has the highest known theoretical charge capacity. Current Si anodes, however, suffer from early capacity fading caused by pulverization from the stresses induced by large volumetric changes that occur during charging and discharging.

An innovative system aimed at resolving this issue is being developed. This system incorporates a thin Si film bonded to an elastomeric substrate which is intended to provide the desired stress relief. Non-linear finite element simulations have shown that a significant amount of deformation can be accommodated until a critical threshold of Li concentration is reached; beyond which buckling is induced and a wavy structure appears. When compared to a similar system using rigid substrates where no buckling occurs, the stress is reduced by an order of magnitude, significantly prolonging the life of the Si
anode. Thus the stress can be released at high Li-ion diffusion induced strains by buckling the Si thin film.

Several aspects of this anode system have been analyzed including studying the effects of charge rate and thin film plasticity, and the results are compared with preliminary empirical measurements to show great promise. This study serves as the basis for a radical resolution to one of the few remaining barriers left in the development of high performing Si based electrodes for Li-ion batteries.
To my fiancé and future wife, whose love and encouragement have helped me to
overcome so many obstacles in order to achieve so much.
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CHAPTER 1

INTRODUCTION AND REVIEW OF LITERATURE

1.1 Motivation for Research

Many top researchers are continuing to focus on some of the greatest challenges for our society today, one of which is producing reliable and renewable energy that will promote economic development and independence while lessening environmental impacts for future generations. Most energy systems today require a steady power supply, however many renewable energy sources, such as solar energy, alone cannot provide this continuous supply throughout the day and night. Therefore it is critical that efficient means of storing energy be developed in order to transform abundant renewable energy into an on-demand source of power for other sustainable technologies. In fact the wide-scale use of some green technologies such as electric vehicles has been slowed due to insufficient means of storing enough portable energy (Armand and Tarascon 2008). The development of energy storage devices with high energy/high power density will contribute to the number one “Grand Challenges for Engineering” in the 21st century of “making solar energy more economical,” as stated by the U.S. National Academy of Engineering ("Grand Challenges for Engineering" 2010). The number of viable energy storage devices continues to grow, and Lithium (Li) ion batteries, a relatively new storage medium, are seeing a slow stream of improvements as they are introduced into many consumer electronics, electric vehicles and aircraft, and medical devices. Li-ion batteries are well suited for portable or off-grid applications, such as environmentally
friendly electric vehicles, because of their high energy-to-weight ratios, high energy densities, and reasonable life cycle. Despite the immense demand for Li-ion batteries, the progress of battery technologies as a whole has been typified as much slower than the electronic devices they are meant to power.

Current research into Li-ion batteries is focused on improving the battery’s performance by enhancing its energy (power) density. By changing the electrode materials, greater energy capacities for these batteries can be realized. Silicon (Si) as an anode material has been extensively studied because it has the highest known theoretical charge capacity; over ten times that of conventional graphite-based anodes. Current Si anodes, however, suffer from early capacity fading caused by pulverization, a result of the large volumetric changes that occur during charging and discharging (Boukamp, Lesh, and Huggins 1981). Therefore in order to utilize the high performing Si anode effectively, the challenge of obtaining cyclic stability of the material by relieving the stress in the Si itself must be overcome. Thus, the bottleneck of the development of Si anode Li-ion batteries is actually a mechanics problem.

1.2 Li-Ion Battery Background

In terms of rechargeable batteries, Li-ion batteries are the most popular and state of the art portable energy storage device. These batteries can boast one of the best energy-to-weight ratios, lower maintenance requirements, and higher operating voltages (Tarascon and Armand 2001; Teki et al 2009). Li-ion batteries dominate three segments of the market which include: (1) consumer goods such as portable computers, cell phones, cameras, etc., (2) commercial or industrial
products such as vehicles, medicinal products, equipment for railroads, telecommunications, water services, wind and solar power, etc., and (3) special purpose products for research and the military (Kedrinsky and Pashikov 2002). In light of its success, the Li-ion battery is still not at its full potential. There are numerous areas in the design of these batteries where extensive improvements can be made to enhance its overall energy capacity. This section will set the stage for discussing one of the most important of these improvements by first explaining how the Li-ion battery operates in very general terms as well as provide a brief account of the history of Li-ion battery development.

Batteries in the most basic sense are composed of two electrodes (a cathode and an anode) contacting an electrolyte. Rechargeable Li-ion batteries operate on the "rocking chair" principle, whereby the electrolyte transfers Li-ions (but not electrons) between the two electrodes reversibly during charging and discharging (Figure 1.1). The introduction of positively charged Li-ions into a host structure causes electrons to migrate from the host to the current collector. The electrons then flow through circuitry to power the device it is connected to. The cathode is considered to be the positive electrode, which accepts Li-ions during discharge of the battery and releases Li-ions during charging. The anode is the negative electrode, which operates in the opposite sense as the cathode. A separator is placed in the electrolyte to isolate the two electrodes from each other while permitting Li-ions to pass through.
It is commonly believed that interest in lithium-based batteries formerly began in 1958 with W. S. Harris who published a thesis focused on propylene carbonate systems (Schalkwijk and Scrosati 2002; Pistoia 1995). It was not until the 1970s that development and initial commercialization of primary (non-rechargeable) lithium batteries became a major factor in the portable energy market. Most of these systems used metallic lithium or lithium alloys for both the positive electrode (cathode) and the negative electrode (anode). Using lithium, which is the lightest weight, has the highest voltage capacity, and has the greatest energy density of all metals (Schalkwijk and Scrosati 2002), in battery designs was a great leap forward, however the safety issues involved with the unsafe electrical heating of the Li metals causing fires. Explosions were sometimes observed using metallic lithium with liquid electrolytes due to dendritic Li growth during battery operation (Tarascon and Armand 2001). The cause for this hazard is due to the reaction between electrodeposited Li and certain electrolytes, and it
caused many concerns for public use and dozens of recalls (Pistoia 1995). The safety concerns along with the desire to develop a rechargeable Li battery motivated scientists to push for further improvements.

The 1970's and 1980's saw much work on secondary (rechargeable) Li battery electrodes. Initially secondary batteries used Li insertion compounds, the most famous being Li/MoS$_2$ developed by Moli Energy Ltd., as the cathodes and metallic Li for the anodes, yet the safety issues were not resolved and the reversibility of the process was rather poor (Schalkwijk and Scrosati 2002). It was discovered that Li-ions could be reversibly intercalated into several host compounds for use as both electrodes in secondary Li batteries (Pistoia 1995), thus the Li-ion battery was created. Intercalation in terms of chemistry refers to the incorporation of a foreign atom into another crystal's lattice, usually at the interstitial locations (Kedrinsky and Pashikov 2002). One of these host compounds that proved to be invaluable in the development anodes within rechargeable Li-ion batteries is carbon materials, in particular graphite. Many researchers began studying carbon as an anode for Li-ion batteries (Steele 1971; Armand 1980; Goodenough and Mizuchima 1981) after it was found that carbon could easily exchange Li-ions reversibly (Tarascon and Armand 2001). Li can be intercalated into graphite in a ratio of one Li to six carbon atoms at the interstitial sites (Figure 1.2) between A-A stacking of carbon sheets. Using a cathode made of a Li alloy that can intercalate and de-intercalate Li-ions as well will generate what is known as the "rocking chair" effect for the battery cell. Thus there is no
metallic Li present, only Li-ions that travel between the two electrodes via the electrolyte, thus improving the safety of the battery (Tarascon and Armand 2001).

![Lithiated graphite, LiC₆, structure](image)

Figure 1.2 Lithiated graphite, LiC₆, structure (Courtesy of Pistoia 1995).

In 1991 Sony introduced and commercialized a secondary C/LiCoO₂ Li-ion battery (Figure 1.1) which serves as the foundation for today’s rechargeable Li-ion batteries (Nagaura and Tozawa 1990). The demand for Li-ion batteries has been driven by the portable electronics market, which has seen profound growth as improvements to current products are being made and as new devices are being introduced (Armand and Tarascon 2008). More powerful electronics are requiring increasingly more potent energy sources. Unfortunately, the development of portable power sources has seen only marginal growth (Broussely and Archdale 2004), although not for a lack of effort. An incredible amount of work involving the chemistry, materials, design, and manufacturing has been performed to enhance the performance of Li-ion batteries (Schalkwijk and Scrosati 2002), but the design remains relatively the same over the past 20 years, only increasing in energy density by 8 or 9% (Chiang 2010).
1.3 Recent Research of Si Anodes

Research into the area of Li-ion batteries focuses on developing a cell with greater power and energy density and with improved cycle life. A big part of this research involves developing new materials for the electrodes, separators, electrolytes, etc. Other activities include implementing different alloys and using additives to the electrodes to lower cyclic losses or to improve adhesion to current collectors. Regarding the cathode, many transition metal phosphates such as LiFePO$_4$ (Kang and Ceder 2009) or spinels such as LiMn$_2$O$_4$ (Whittingham 2004) are being researched as replacements for the LiCoO$_2$ electrode. Improving the anode however will provide more gains in overall battery capacity and life cycle improvements. While the specific insertion capacity of the carbon anode is 372 mAh/g (Teki et al 2009), which when used in Li-ion batteries produces a cell capacity that is comparable to similar metallic Li batteries but is much more stable and is reversible; there are many materials that have inherently higher capacities. The material with the highest insertion capacity of 4,200 mAh/g (Kasavajjula, Wang, and Appleby 2007; Teki et al 2009), over an order of magnitude higher than carbon, is silicon (Si). Si can reversibly intercalate Li-ions, has an outstanding energy capacity, and it is the second most abundant element on the planet (Boukamp, Lesh, and Huggins 1981). Because of these facts, many researchers have vigorously attempted to utilize Si in several forms as anodes for Li-ion batteries.

The biggest problem experienced with Si as anodes is the extremely large volumetric expansion and contraction that occurs during lithiation and delithiation
respectively. Specifically, each Si atom accommodates 4.4 Li atoms which forms the cubic Li$_{22}$Si$_5$ alloy (Sharma and Seefurth 1976; Marel, Vinke, and Lugt 1985). This is the reason for the 400\% volume expansion experienced by the host Si lattice (Boukamp, Lesh, and Huggins 1981). This causes the Si anode to self-pulverize after one a few cycles; disintegrating itself (Figure 1.3) causing a severe drop in capacity due to reduced electric contact. For example, bulk Si anodes experience a 65\% drop in capacity after the first cycle (Ryu et al 2004). Thus the aspect of Si that makes it so attractive as an anode material is also the biggest obstacle in practically implementing the material. In response, scientists and researchers have tried many different approaches to work around this feature of Si anodes. The most promising results have come from work regarding Si nanostructures. Si nanostructures for use as anodes can take advantage of large surface-to-volume ratios and short diffusion lengths for greater power-density (Zhao et al 2008). Nanostructures can also survive larger stresses without failing because their small dimensions limit the size of precursor cracks when compared to bulk materials (Teki et al 2009). Therefore Si nanostructures have become very attractive possibilities for anodes in the next generation of Li-ion batteries.

Figure 1.3 Diffusion-induced stress pulverizes the Si during cyclic charge and discharge causing loss of electrical contact.
1.3.1 Si Nanoparticles

Nanoparticles (i.e. very fine powders) of Si would serve to reduce overall volumetric expansion and subsequent disintegration (Kasavajjula, Wang, and Appleby 2007), however by themselves they cannot serve as anodes because they would lack any connectivity amongst themselves. Using pure Si powder anodes that are compressed into a bulk form suffer from poor cycle life and highly irreversible capacity due to the loss of contact between particles during delithiation (Kasavajjula, Wang, and Appleby 2007). Thus research has been done to place Si powders within a matrix host material that serves as a cushion for the particles as they expand and contract (lithiation and delithiation). The matrix material itself can be either inactive (does not intercalate Li-ions) or active (will accept Li-ion insertion/removal to assist the battery operation).

An inactive matrix is usually metallic such as TiN (Kim, Kumta, and Blomgren 2000) or TiB$_2$ (Kim, Blomgren, and Kumta 2003). In general the matrix material must have a high strength to endure the large volume change of the Si particle as well as highly conductive to permit the charge transfer during electrochemical reactions. The anodes are fabricated by milling Si powders with the inactive material to a desired size, followed by mixing them with solutions of polymers such as polyvinylidene fluoride (PVDF) to act as a binder. The mixture is turned into a slurry which is deposited as a film onto a metallic film which doubles as a current collector within a battery test cell that uses Li foil as the cathode and a reference. It was found in the aforementioned studies that the matrix did act as a cushion because the morphology was relatively unchanged.
after cycling, however the specific capacity was rather low (ranging between 300 to 500 mAh/g at 10 cycles) but stable after an initial fade (Kim, Kumta, and Blomgren 2000; Kim, Blomgren, and Kumta 2003). Thus these anodes did improve the cyclic stability trouble with bulk Si, however the specific capacity is too low for commercial applications. The low reversible capacity is likely due to poor Li-ion diffusion through the matrix, limiting the number of reactions between Li and Si.

An active matrix will support the Si in the intercalation of Li-ions. Metallic materials such as silver or magnesium could be used, but the most prevalent active material used is carbon. Carbon is relatively soft, and has low density but excellent electrical conductivity. Again the Si powders are milled with the matrix material which this time is either graphite flakes (Liu et al 2005) and/or carbon black (Li et al 1999). In a different study (Wang et al 2004), a carbon aerogel was synthesized with Si powders stirred in it. In other studies the ball milling was combined with chemical/thermal vapor deposition (Kasavajjula, Wang, and Appleby 2007). Another study used Si coated in carbonous shells within a soft matrix (Zhao et al 2008). Mixed with a polymer binder as well, the Si materials dispersed in the carbon matrix materials are placed on metallic foil and then put within a battery test cell. A stable capacity as high as 1,500 mAh/g was observed (Liu et al 2005; Wang et al 2004), however the capacity was highly dependent upon Si size and the concentration of the Si and the matrix material. In some studies degradation of the anode was observed due to the loss of contact during delithiation resulting in voids (Wang et al 2004), which is likely due to the
different diffusion characteristics between the Si and carbon material. The use of Si-core carbon-shell nanocomposites also improved the cyclic stability by preventing aggregation of Si particles, however its performance barely surpassed that of graphitic anodes (Zhao et al 2008).

Using matrix materials serves to cushion the expansion of Si powders during the intercalation of Li-ions. Improvements in cyclic stability compared to bulk Si (which only survives 5 to 10 cycles or so) have been shown; however the aforementioned studies do not go to a very high number of cycles. Inactive materials promote cyclic stability but have limited capacity. They also incur excess weight penalties. Active materials (carbon) also improve the stability of the anode while increasing the specific charge capacity above that of graphitic anodes by intercalating the Li-ions simultaneously with the Si particles. A likely pitfall of these types of anodes is performance fading that could occur due loss of electric contact due to the stress caused by Si expansion and contraction (Kasavajjula, Wang, and Appleby 2007; Zhang et al 2008).

1.3.2 Si Films

Due to the improved reversibility and capacity retention seen for Si particle nanocomposites, attention was turned to other nanostructures. One such structure used was Si thin films. These films, either crystalline or amorphous, are usually created via deposition techniques and do not have the inactive binding materials or additives that are present in the nanocomposites. Attempts at understanding the mechanism of Li insertion and extraction in Si films resulted in the discovery that the crystal structure of pure Si changed to an amorphous phase.
upon lithiation and recrystallization, albeit not full recrystallization, upon
delithiation (Li et al 2000). Both crystalline and amorphous Si can achieve
similar specific capacities however (Cui et al 2009a). The large volumetric
expansion caused neighboring Si particles to agglomerate, which reduced the
local Li insertion/extraction kinetics causing capacity fade and shorter cycle life
(Kasavajjula, Wang, and Appleby 2007). Thus the primary objective of studies of
Si films is to prevent this clustering of Si caused by the phase change.

It was found that the thickness of an amorphous Si film on metallic foils
played a major role in the lithiated Si structure, with thinner films down to
hundreds of nanometers or less experiencing no crystalline phase formation
(Hatchard and Dahn 2004) and less electrical resistance (Yoshimura et al 2005).
The performance of a Si thin film anodes depended on the uniformity of the film,
with the best results of 2,000 mAh/g at 50 cycles and 1,500 mAh/g at 700 cycles
(Ohara et al 2003). Additionally, amorphous Si appears to have a greater cyclic
performance than crystalline Si (Ohara et al 2003; Maranchi, Hepp, and Kumta
2003), therefore amorphous Si is used most prevalently. Other factors that helped
to improve the capacity fade of Si thin films include doping which enhanced the
Si conductivity (Ohara et al 2003; Takamura et al 2004; Yoshimura et al 2005)
and increasing the adhesion between the film and the current collector (Zhang et
al 2008; Takamura et al 2004). The adhesion is typically increased by roughing
the surface of the current collector. Some researchers sought to use films that
could accommodate large volumetric changes and thus developed short Si pillar
arrays (810 nm thick with average diameter of 580 nm) on Si substrates fabricated
using island lithography (Green et al 2003) and porous Si films (with pores as large as 1 \( \mu \text{m} \) diameter) fabricated by electrochemical etching (Shin et al 2005). The pillars featured good cyclic stability and capacity retention, but low efficiency (70%) at 40 or more cycles (Green et al 2003). The porous Si films suffered from heavy degradation after about 35 cycles due to disintegration originating at Si lattice defects (Shin et al 2005). An effort was made to deposit a film atop a nanostructures compliant layer of tilted copper (Cu) nanorods (Karabacak et al 2004; Karabacak et al 2005), as a means of preventing stress build up in the Si film. This attempt, however, suffered from delamination between the Si film and Cu nanorods and failure of the Si film between the nanorods. The authors proposed that a low modulus interface between the Si and Cu should be used in order to mitigate the stress in the film (Karabacak et al 2004; Karabacak et al 2005).

Si thin films deposited on current collectors have shown better reversible capacity, capacity retention, and long cycle life when compared to the Si particle nanocomposites, most likely due to the absence of inactive materials, the greater stability, and better adhesion to current collectors (Kasavajjula, Wang, and Appleby 2007). Some thin films Si anodes can obtain specific capacities up to 2,000 mAh/g for a duration of hundreds of cycles. Despite the benefits of the thin films, it was observed that the films would sometimes break up into smaller portions that would eventually delaminate from the current collector (Teki et al 2009). Thus fracture is not avoided by using thin films. The fabrication of Si thin
films via deposition means is often very costly, which limits its practicality in commercial cells (Kasavajjula, Wang, and Appleby 2007).

1.3.3 Si Nanowires

Recently a group at Stanford University developed Si anodes made of aligned Si nanowires (NWs). The fundamental assumption behind using Si NW is that they can accommodate the large volumetric changes without the use of binders. The NWs are grown via vapor-liquid-solid (VLS) methods in arrays directly on a stainless steel substrates such that all NWs are connected to the current collector. These Si NWs have excellent discharge capacities as high as 3,200 mAh/g at 10 cycles; a high performance that is attributed to the facile strain relaxation (Figure 1.4) which preserves the NWs from breaking into smaller pieces, short, one-dimensional diffusion paths, and also the direct contact of each NW with the current collectors (Chan et al 2008). After charging the Si NW morphology is observed to change irreversibly, becoming an amorphous material with a larger diameter and a textured surface (Chan et al 2008). After 20 cycles the capacity off the Si NWs was 75% that of the theoretical maximum of Si (Chan et al 2008; Teki et al 2009).

![Facile relaxation](image)

Figure 1.4 A schematic demonstrating the facile strain relaxation of Si NWs
Si core-shell nanowires have also been studied where the shell is an amorphous Si material and the core is either a crystalline Si (Cui et al 2009a) or carbon nanofibers (Cui et al 2009b). These nanostructures have demonstrated approximately 90% or better capacity retention and a specific energy capacity of roughly 1,000 mAh/g (Cui et al 2009a; Cui et al 2009b). Like the Si NWs, these core-shell NWs also can endure high charge and discharge rates at reasonable discharge capacities (Chan et al 2008; Cui et al 2009a; Cui et al 2009b). A heavy loss in reversible capacity is incurred after the first cycle for these nanostructures, which the authors, unlike many others, do not attribute to surface passivation and the formation of a solid electrolyte interphase (SEI), rather they believe it is due to unknown mechanisms that require further study (Chan et al 2008).

The use of Si NWs has shown that very high specific capacities are attainable. The large volumetric changes during lithiation and delithiation are accommodate by virtue of the Si NW geometry and good contact with the current collector is maintained, both of which are attributed to the anodes performance. Dimensional changes in length and diameter are observed in the NWs themselves after cyclic lithiation consistent with the reported 400% increase (Chan et al 2008). The experimental results for these nanostructures only show the performance of the anode up to tens of cycles. Thus the long life stability over hundreds of cycles is as yet unknown.
1.3.4 Summary

Significant gains have been made in terms of cycling retention and energy capacity of Li-ion batteries by utilizing different Si nanostructures instead of bulk Si. Early attempts to use Si nanocomposites showed that indeed an anode with Si constituents could be stable, however the resulting capacity is not high enough to warrant replacement of current carbonous anodes. Si films along with Si nanowires have shown very good improvements in most respects to the anode performance, however the use of these two structures seems to circumvent the issue of Li-ion diffusion induced stress. Si NWs allow for facile strain relaxation, however the Si material's stress state and its behavior under lithiation and delithiation is not well understood. As such there are limits to these structures, suggesting that employing nanostructured Si anodes by themselves may not fully resolve the stress issue. Thus it is critical to develop an innovative approach that will relieve the diffusion-induced stress and to subsequently understand the underlying mechanisms.

1.4 Thesis Overview

This thesis aims to be the first steps in the study of a potential Si anode system designed to resolve the diffusion-induced stress issue. The stress relaxation concept is analyzed by use of the finite element (FE) method to substantiate initial hypotheses and to provide a fundamental understanding of how stress relaxation may be obtained. This section outlines the objectives and contributions of this work. It will describe the goals of the work, and provide brief synopses of each chapter contained in this thesis.
1.4.1 Hypothesis

The idea of stress relaxation for Si anodes stems from recent work regarding controlled buckling of stiff, Si films on soft, elastomeric substrates for use in many applications (Khang et al., 2006; Sun et al., 2006; Kim et al., 2008a; Yu et al., 2008; Yu et al., 2009; Yu et al., 2010; Ko et al., 2008). Buckling, in a traditional sense is considered to be a catastrophic failure of a structure; however researchers have shown that buckling can be used to great advantages. The biggest advantage in terms of stress relief is that large deformations accompanied with relatively small stress can be obtained from a buckled structure bonded to soft substrates.

Thus it is proposed that the same mechanisms can be applied to Si anodes for Li-ion batteries. It is conjectured that a flat, Si film on a soft substrate will be relatively free to expand, and nearly stress-free during lithiation. The constraint of rigid substrates (i.e. current collectors), will be replaced by a compliant medium that only minimally restricts the expanding Si. Therefore it is believed that the diffusion-induced compressive stress, caused by large volumetric expansions in Si, will be reduced when compared to traditionally rigid substrate systems, and that subsequent buckling (Figure 1.5a) due to the eventual development of stress above a critical limit will provide a means of cyclic stability, acting like a spring during the lithiation and delithiation of the Si anode (Figure 1.5b). The soft substrate that is to be used is poly(dimethylsiloxane) (PDMS), a very common elastomer used in research. The goal of the proposed
research is to provide the theoretical understanding of this stress relaxation mechanism using numerical simulations on the continuum level.

Figure 1.5 A schematical demonstration of (a) the initial buckling caused by buckling of Si on soft substrates and (b) the cyclic benefits of us buckled Si films on soft substrates as anodes.

1.4.2 Summary of Thesis Chapters

Chapter 1 has provided a brief background regarding the operation and history of Li-ion batteries. In order to produce the next generation of high performing batteries new electrodes need to be developed that utilize high capacity materials. The best opportunity to expand the energy capacity of Li-ion batteries is to employ Si as an anode because of its highest known specific energy capacity. Bulk Si, however, suffers from early capacity fading due to self-pulverization during cyclic charge and discharge. Recent research to implement Si nanostructured anodes into Li-ion battery test cells have been discussed, showing that improvements in anode performance can be made by circumventing the stresses that cause disintegration. The major goal of this thesis is to study a novel Si-soft substrate system that will relieve the stress caused by Li-ion insertion.
Chapter 2 begins with an introduction to the FE method. Then several models of increasing complexity are presented. Each model describes the same trend in terms of the Si film on soft substrates: buckling does indeed occur, but not after a significant amount of lithiation strain. This buckling of the thin film into a smooth, wavy shape on a soft substrate leads to a large decrease (by an order of magnitude) in the Si stress when compared to an equivalent system that has a rigid substrate. The buckled morphology is characterized in the numerical simulations as well. It is found that the wavelength is relatively constant after buckling while the amplitude increases gradually. This increase in amplitude is understood to be the reason for post-buckling stress increases.

After the modeling techniques are established in Chapter 2, Chapter 3 looks into the effects that charge rate may have on the Si anode on soft substrates. It is found that homogeneous diffusion through the Si thickness is the most desirable case in order to take full advantage of the benefits provided by the soft substrate. From the perspective of nanostructures, this uniform diffusion is quite plausible given their short diffusion lengths.

All of the analyses demonstrated thus far used linear elastic material models, however it has been recently determined that plastic flow occurs during lithiation and delithiation. This plastic behavior is a new discovery for Si anodes, and as such very little is known about it at this time. Thus Chapter 4 seeks to qualitatively determine how this plastic behavior will affect the stress relaxation and the buckled morphology. The transition from elastic to plastic causes a shift in wavelength, thus the analysis provides evidence that a fundamental relationship
between the moduli of the film and substrate controls the buckled morphology. This change in morphology has some interesting implications on the stress state of the Si thin film.

Chapter 5 provides a brief look into preliminary experiments that have been performed. These experiments confirm the thesis hypothesis. An anode made from Si in the form of ribbons (created by silicon-on-insulator wafers) that is bonded to a soft PDMS elastomer along with a gold and chromium current collector is fabricated in an enert environment. Thus a Si-PDMS anode system is created. After cyclic testing in a battery test cell, the results prove to be excellent. The cyclic discharge capacity retention is 85%, reaching approximately 3,500 mAh/g after 500 cycles. This specific capacity is higher than the nanostructures studied in the field thus far. The Si ribbons indeed buckle which is believed to be the cause for the excellent stability of this Si anode system.

Finally, the entire thesis is summarized in Chapter 6. The FE analyses performed are summarized along with a brief discussion of the experimental results. Conclusions and recommendations for future work are discussed as well.
CHAPTER 2

STRESS RELAXATION OF SILICON ANODES

2.1 Introduction

The first objective of this study is to ascertain the feasibility of accomplishing stress relaxation of the Si anodes by using soft substrates. This is a very important step, for once good prospects for stress relaxation are determined a more rigorous study of the Si-PDMS anode system can be performed. This first look is done using computational tools. A simple FE model is created as a means to test initial assumptions and determine the best course for future analysis. It is found that at a critical stress/strain the diffusion of Li-ions in the Si material will induce a wavy, buckled shape to appear in a thin Si film when bonded to a soft, PDMS substrate. This buckled morphology is created because compressive stresses build (slowly) in the film due to the constraint applied by the soft substrate, until a critical point is reached where Si structure becomes unstable and releases its strain energy by wrinkling. Further complexities and refinements can then be made to this model in order to evaluate and/or reduce these assumptions and to also analyze more intriguing behavior of this novel Si-anode system. The focal point of the initial and all subsequent simulations is, of course, the evolution of stress within the Si material, however parameters regarding the film's morphology such as wavelength and amplitude will also be measured.

2.2 The Finite Element Modeling and Abaqus

The finite element method (FEM) is a numerical technique designed to produce approximate solutions to often complicated engineering problems where
closed-form solutions of complex differential equations are difficult or impossible to obtain (Lepi 1998). The FEM is used predominantly for structural mechanics and heat transfer analysis (MacNeal 1994), however other areas of engineering such as fluid mechanics, mass transport, and electromagnetics are able to utilize the FEM as well (Logan 2002). The general procedure is to divide (mesh) a continuum into many smaller domains called "finite elements" that are connected to each other or to the boundaries at "nodes," and to then solve a system of equations for the elements instead differential equations for the entire, complicated body. Solving any structural problem involves satisfying three fundamental requirements: equilibrium, compatibility, and constitutive behavior (NAFEMS A Finite Element Primer 1992). The science behind the FEM is the various methods it employs to solve the system of equations for the elements of the model. The art of the FEM includes the choice of appropriate elements, the element size, the order of the elements, appropriate loading and boundary conditions, load incrementation, etc.

Abaqus, a SIMULIA product, is one of several commercially available finite element packages. This trusted and efficient software is capable of solving numerous linear, non-linear, and perturbation analyses and is accompanied with an extensive library of elements, a variety of elastic and inelastic material definitions, and a host of special constraints/interactions ("Abaqus Unified FEA" 2010). For this study Abaqus version 6.7-1 is used to perform simulations on the Si-PDMS anode system. In particular, Abaqus's linear perturbation and nonlinear solvers will be employed for this study. It is important to remember that Abaqus
processes simulations in "unit-less" format, thus the user is responsible for maintaining a consistent set of units for input data and for extracting data. Abaqus uses numerical techniques to integrate quantities over the elements' volume, thus it is able to be generally solve a problem without depending upon the material behavior (Abaqus Analysis User's Manual 2007).

Using the displacement-based finite element formulation, Abaqus satisfies the equilibrium condition in its "weak form" by using the principle of virtual work,

\[ \int_{V} \sigma : \delta \varepsilon \, dV = \int_{s} t \cdot \delta u \, dS + \int_{V} f \cdot \delta u \, dV \]  \hspace{1cm} (2.1)

where \( \sigma \) is the stress measure, \( \delta \varepsilon \) is the virtual measure of strain rate, \( t \) is the surface traction, \( f \) is the body force, and \( \delta u \) is a virtual displacement field (or any other test function). The strain measure used depends upon how the selected element is formulated (Abaqus Theory Manual 2007). Once the body is meshed into many elements, an interpolation function (a continuous, polynomial function) is used to describe the element's behavior at and between its nodes,

\[ u(x, t) = N(x)q(t) \]  \hspace{1cm} (2.2)

where \( N(x) \) is the shape function and \( q(t) \) is the nodal degree of freedom vector (displacement, rotation, etc.). Thus in essence the continuous function (continuous body) is discretized into many polynomials (elements). The nodal displacements and rotations must be kinematically admissible, i.e. consistent with the boundary conditions. The strain is related to the nodal displacements via the interpolation assumption.
\[ \varepsilon(x, t) = B(x)q(t) \]  

(2.3)

where the \( B(x) \) is a function of the geometry and the shape functions. The constitutive relationship is satisfied according to

\[ \sigma(x, t) = D\varepsilon(x, t) \]  

(2.4)

where \( D \) is a positive definite material matrix. Substitution of equation (2.2) - (2.4) into equation (2.1), neglecting body forces, and manipulating the result yields a system of equations of the form

\[ Kq = F \]  

(2.5)

where

\[ K = \int_V B^TDBdV \]

is the stiffness matrix of a single element (the local stiffness matrix) and

\[ F = \int_A N^T \cdot tdA \]

is the applied force array. As will be elucidated in further sections, a thermal stress analysis will be performed. In this case the force array is represented as

\[ F = \int_V B^TDe_TdV \]

where \( e_T \) is the applied thermal strain (Logan 2002). Inertial effects can be considered by introducing body forces according to equation (2.5) Newton's Second Law to produce
\[ \mathbf{K}\mathbf{q} + \mathbf{M}\ddot{\mathbf{q}} = \mathbf{F} \]  \hspace{1cm} (2.6)

where

\[ \mathbf{M} = \int \rho \mathbf{N}^T \mathbf{N} \, dV \]

is the mass matrix and \( \rho \) is the material density. Note that the *global stiffness* matrix is the assemblage of all the local stiffness matrices when solving the entire model (Buchanan 1995). Solving a linear problem using FE analysis is done by solving the set of global equations for all elements described by equation (2.5) or (2.6) for the entire model. Solving nonlinear problems involves a "time" incrementation history whereby equation (2.5) or (2.6) is solved at each discrete increment (a fraction of the entire load). Abaqus has many numerical techniques to march through the history until a final converged solution is obtained, the most familiar being Newton's method (Abaqus Theory Manual, 2007).

2.3 Analysis Procedure

The FE model for the Si-PDMS anode system itself is very simple in its construction. The anode system is modeled inside a 2-dimensional (X-Y plane) framework as a very thin structure placed atop a very thick one (Figure 2.1). Both structures are bonded together in order to maintain contact throughout all simulations. The model is designed to be a realistic representation of a feasible Si-PDMS anode system. This approach is an efficient means (compared to a full 3-dimensional analysis) to test the concept of stress relaxation by buckling while expediting the time to achieve a converged solution.
The analysis procedure can be divided into 4 distinct steps (Figure 2.2). The first step includes all pre-processing activities such as model creation, material property assignment, element selection, meshing, etc. The second step is an elastic buckling analysis of the model via a perturbation of the system. This type of analysis is carried out via eigenvalue extraction of a linearly perturbed system, where the eigenvalues are multipliers of the applied loads (Abaqus Theory Manual 2007). The eigenvalues are thus critical loads which occur at the bifurcation point between a stable and an unstable equilibrium of an ideal-elastic structure (Hibbeler 2005). This type of analysis is consistent with the classic Euler linear buckling solutions presented in many textbooks. The deformed shapes from this step are often referred to as modes. While the results for this type of analysis are generally non-conservative, due to the ideal-elastic assumption, it can provide useful insight into the possible deformed shapes.
Figure 2.2 Flow diagram detailing the four basic steps performed for the simulations of this study: (1) Pre-processing, (2) Linear Buckling, (3) Post-Buckling, and (4) Post-Processing.

The nodal displacements of the modes can be extracted and imported into a second analysis, where a fraction of the deformations are added to the original nodal coordinates. A factor, often referred to as an imperfection factor, is specified which multiplies the deformations before being added to the nodal coordinates. Thus a second model is produced with an intimation of the desired mode as its geometry. This process is used extensively for buckling analyses where geometric imperfections from say manufacturing tolerances or from a desired mode shape are used for further analysis. Thus, the third step, called the post-buckling step, extracts the deformations of a desired mode, applies a very small imperfection to the deformations, and proceeds with further analysis. The post-buckling step is a nonlinear static analysis whereby the model loads are incrementally applied, and equilibrium is assessed at each increment. The objective of this nonlinear analysis is to determine the loading level that will cause a structure to become unstable; thereby finding the actual load of the non-ideal structure at the bifurcation point. Unlike the ideal elastic buckling, a post-buckling analysis can include non-linear material behavior, large deformations,
imperfections, etc. Technically speaking, "post-buckling" occurs after the critical point where the structure turns unstable, however for all intensive purposes this step is a single analysis, thus it will be termed the post-buckling step in its entirety.

The fourth and final step includes all post-processing activities of the post-buckling step; which include extracting nodal and element results, such as forces, strains, stresses, etc, and generating contour plots for variables of interest. The key features that will be analyzed from the post-buckling step include the evaluation of stresses within the Si material and the measurement of the resulting wavelength and amplitude.

2.4 Proof of Concept

As a first step, a finite element model using simple elements and materials is created. The goal of this initial simulation is to demonstrate a proof of concept for the stress relaxation mechanism by providing invaluable data regarding the response of the system. Thus no rigorous study of the underlying FE principles will be done; rather it is saved for later on. This model is used to illustrate how the Si thin film deforms due to the expanding lattice caused by Li-ion insertion.

A flat, 100nm thin silicon film is created within the software and it is then perfectly bonded to a very thick PDMS substrate. The thickness of the substrate is over three orders of magnitude larger than that of the film. The bonded condition is achieved by utilizing a “tie” constraint between the neighboring nodes of the film and the substrate. This constraint couples the degrees of freedom of the interfacial nodes between the film and the substrate, which ensures
that the film-substrate interface remains intact. The nodes that belong to the Si and those belonging to the substrate are distinct, yet coincident, thus by tying their translational degrees of freedom no artificial moments are created by nodal location mismatch when bonding elements with rotational degrees of freedom to elements that have no rotational degrees of freedom (Abaqus Analysis User's Manual 2007).

The elements that make up the film are assigned with properties of an isotropic elastic silicon material, $E = 130$ GPa and $\nu = 0.3$ (INSPEC 1988; Wortman and Evans 1965; Callister 2007) with a coefficient of thermal expansion (CTE) of $2.6 \cdot 10^{-6} \, ^{\circ}C^{-1}$ (Tokumaru and Okada 1984; Callister 2007). Silicon is a cubic crystalline material (Kasavajjula, Chunseng, and Appleby 2007) thus it has some degree of anisotropy, however upon lithiation the Si-Li material becomes amorphous after the first charge (Chan et al 2008). These amorphous properties are unknown, thus the silicon material is assumed to be isotropic with the aforementioned properties for the purposes of this study. The substrate is assigned the isotropic elastic material constants for PDMS. The elastic modulus of PDMS is set at a constant 2 MPa and its Poisson's ratio is 0.495 for all simulations (Bietsch and Michel 2000; Lotters et al 1997; Govindaraju, Chakraborty, and Luo 2005). PDMS is a material that can range in its viscoelastic performance depending upon its fabrication, cross-linking, molecular weight, etc. It is possible to obtain PDMS with very weak viscoelasticity, such that its loss modulus is very small and the storage modulus is approximately 2 MPa (Young's
modulus). Thus for the purposes of this analysis, a weak viscoelastic PDMS is assumed in order to use the aforementioned linear elastic material properties.

Initially the Si material is represented using beam elements (element B21 in Abaqus) which are one dimensional in formulation and are especially good at accurately capturing bending phenomena, prevalent in buckling occurrences. The B21 elements are composed of 2 nodes with two translational and one rotational degree of freedom and are linear in formulation. They follow the Timoshenko theory for beams (Abaqus Analysis User's Manual 2007), however due to the slenderness of the Si film, both Timoshenko and Euler-Bernoulli theories yield equivalent results. Beam elements are assigned values for their cross-sectional areas and area moments of inertia both of which depend upon the film thickness. The PDMS substrate is considered to be plane strain (CPE4R elements with two translational degrees of freedom); a very long, prismatic structure such that out-of-plane deformations are negligible.

The geometry of the system presents a significant computational challenge regarding the total number of degrees of freedom. In particular a fine mesh of the Si material is required in order to sufficiently capture the deformations due to buckling. Because of the large difference in moduli (i.e. abrupt change in stress) between these two materials and because of the aforementioned discussion regarding the coincident nodes at the interface, the substrate must be finely meshed at the interface as well (NAFEMS A Finite Element Primer 1992). The enormous difference in thickness between the Si and PDMS requires a creative meshing scheme in order to reduce the already large number of elements (degrees
of freedom). A general strategy to help reduce the overall number of elements is to partition the substrate into regions of progressively increasing element size starting from the finely meshed interface (Figure 2.3). This approach does not suffer from a lack of accuracy in the coarsely meshed regions (i.e. the base of the PDMS) which are of no interest for this study.

Another challenge with this particular mechanical/continuum simulation is the appropriate representation of diffusion. For the analyses contained herein, Li-ion insertion is represented by using a thermal strain analogy to replicate the strained lattice. This approach has been utilized by several researchers on many occasions, even for Li-ion battery applications (Hu, Zhao, and Suo 2010; Zhang, Shyy, and Sastry 2007). To create this thermal strain a temperature field is applied to the nodes of the Si only. This utilizes another degree of freedom for the nodes apart from their translational and rotational degrees of freedom. The temperature can be considered to be the applied load and it is ramped from zero to the desired point (desired thermal strain) in small increments of the entire step as specified by the user.

The procedure follows the four steps previously discussed (Figure 2.2). For the linear buckling analysis, the left-most node and the right-most node of the film (beam elements) are loaded by a compressive force in order to produce wavy mode shapes (Figure 2.4a). The result of this eigenvalue analysis, the mode shapes, can be tailored by changing the geometric parameters of the model in order to achieve a desired shape. In this way, a symmetric and periodic wavy
Figure 2.3 A schematic detailing (a) a sample partitioning strategy for the substrate and (b) the resulting mesh.

shape is produced (Figure 2.5). It is advantageous to use a mode that is similar to the expected post-buckling morphology. Thus some knowledge of the final structure (either from experience or trial and error) is helpful. The imperfection factor used for this study is very small (1%), resulting in a second model with a nearly flat film securely bonded to the substrate (Figure 2.5). The loading for the third step is a specified temperature on the nodes of the film to cause a thermal strain which represents a diffusion based strain (Figure 2.4b). Both the eigenvalue buckling (step 2) and the post-buckling (step 3) analyses utilize the same boundary conditions on the substrate. Only the bottom surface of the PDMS is fixed, restricting all planar motion in that region, however the region of the film-substrate interface is not constrained by the user (Figure 2.4). Therefore during the post-buckling analysis the thermal strain will initially cause the film to expand laterally until the substrate begins to constrain this motion.

The thermal load applied to the nodes of the film induces a strain in the elements of the Si material causing lateral deformation (Figure 2.6a). Initially the
soft substrate allows this expansion without much resistance, yet eventually the lateral deformation of the film is restricted as the substrate becomes stretched further (Figure 2.6b). During this time the film elements experience local compressive forces that continually increase in magnitude, however the film remains flat. A critical strain is found to be approximately 7%, where a wavy structure is seen in the deformed shape (Figure 2.6c). At this point, bending moments acting on the film’s elements become evident as the film releases its strain energy by buckling (Jiang et al 2007). The amplitude of the waves continues to increase with higher thermal strain (Figure 2.6d). Upon further straining, more waves appear in the deformed shape (Figure 2.6e-f). The measured wavelength is relatively constant after buckling is initiated due to the lack of constraint in that region. The wavelength is fundamentally dependent
upon the ratio of the film modulus to the substrate modulus and the film thickness (Jiang et al 2007) so it remains constant.

Figure 2.5 A contour plot of deformation from Abaqus showing a mode (symmetric about the centerline) from the linear buckling step and the resulting imperfect shape for the post-buckling analysis.

Figure 2.6 Lateral deformation contour plots showing the evolution of the buckled morphology through the critical strain at (a) 3%, (b) 6%, (c) 7%, (d) 10%, (e) 15%, and (f) 20% strain (same scale).
As noted, the film remains flat until a critical strain is reached after which obvious buckle waves appear. At the onset of the buckling, three distinct waves can be seen in the film with waves propagating as the stress/strain locally exceeds the critical value. In order to qualify trends of the deformed shape, the amplitudes and wavelengths (both normalized by the Si film thickness of 100nm) of these waves are averaged at several strains and reported with errors bars of ±2 standard deviations (approximately 95% of all normally distributed data). Above the critical strain, a sharp increase in the amplitude of the wavy structure is observed (Figure 2.7a). The amplitude is calculated as half of the vertical distance between the peak nodes and their neighboring valley nodes. The trend in the amplitude as a function of the applied thermal strain is one of increasing at a decreasing rate but it is rather linear well after buckling is initiated. It is noted that the amplitudes of the majority of the waves at the center of the model are comparable in magnitude; as seen by the small deviations at higher strains. The distance between the peaks, the wavelengths, is calculated from one peak node to its neighboring peak node. As the applied strain increases, the wavelength remains constant because this part of the model is not constrained by boundary conditions, only the soft substrate (Figure 2.7b). The expansion is permitted and rather than shift in wavelength, more waves propagate down the film’s length as the elements at the periphery reach their critical stress. In general the deviation of the wavelength is greater than that of the amplitude primarily because the Si thin film is discretized down the length with beams (the direction where wavelengths are measured). Since the wavelengths are measured from node-to-node at the wave
peaks, there may exist a variation of up to one element’s width for wavelength measurements depending upon the morphology at a particular increment.

Figure 2.7 Measured values, normalized by the Si thin-film thickness, for the buckled morphology of (a) amplitude and (b) wavelength with ±2 standard deviation error bars.

As it was shown in the contour plots of deformation and the graphs of amplitude and wavelength, the plot of stress as a function of the applied strain (for the middle element of the film, which experiences the largest magnitude of stress and thus buckles first) indicates a critical strain of 7% as well (Figure 2.8a). Before the critical strain is reached, the stress remains exclusively compressive. Upon buckling after 7% strain, the elements experience a local bending moment (Figure 2.9a) which induces a bending stress on the thin film cross-section due to the imperfection. For a single element before buckling, the compressive force builds (Figure 2.9b) until the bending moment begins to manifest itself during the transition from flat to a buckled structure (Figure 2.9c). Two curves are shown to demonstrate that indeed the Si material experiences bending, thus it has a highly compressive zone and a highly tensile zone at the outer fibers. Note the dramatic change in stress once buckling is initiated, due to the sudden introduction of
bending moments (Figure 2.9c). This behavior curbs and turns into a linear relationship between stress and the applied strain.

Figure 2.8 Stress of the Si material demonstrating the introduction of bending stresses at the critical 7% strain: (a) compressive and tensile components of the stress on the beam cross-section and (b) stress relaxation by comparing the stress of the beam cross-section for a stiff (red) and a soft (blue) substrate.

Figure 2.9 Forces and moments on a single element: (a) schematic of forces and moments generated between adjacent elements where, (b) the forces build until the critical strain of 7% whereby (c) a significant bending moment dominates.
If one assumes a fracture stress of 2.6GPa the data from the FE analysis would indicate that failure would occur at approximately 30% of the thermal strain. This stress at fracture would correspond to a crack of characteristic length of 38nm according to the Griffith theory of fracture (Weertman and Evans 1996) using a mode-I stress intensity factor of $K_I = 0.9 \text{ MPa} \cdot \text{m}^{1/2}$ (Ericson Johansson, and Schweitz 1988; Ericson and Schweitz 1990; Callister 2007). A crack feature of this size is almost 40% of the thickness of the host Si material, therefore using the aforementioned fracture stress will be a very conservative estimate. Using the same model but replacing the soft substrate with a stiff one (i.e. using a substrate with stiff Si material properties) will help quantify the amount of stress relief that is obtained by using buckling. Keep in mind that like the previously discussed simulation, the model that has a stiff Si substrate only applies the thermal strain to the elements representing the thin film, thus only the film is “active.” Using a stiff substrate produces very high stresses (Figure 2.8b), since the behavior is almost that of a fixed-fixed condition on the thin film where no buckling occurs. Almost an order of magnitude gap in the stress of the Si material is found at very high strains. Therefore under the conditions of this model, a high degree of lattice strains could be sustained before failure may be observed and the stress is relieved when compared to a Si anode bonded to a stiff substrate.

2.5 Planar Analysis Details

While the study of the Si-PDMS system using beam elements to represent the Si provides an intuitive understanding of how the buckled morphology develops and relieves the stress, there are some limiting assumptions associated
with using the aforementioned elements. In particular the assumption that a beam's section cannot deform in its own plane can be problematic for large amounts of bending. Since the buckling of the Si thin film for stress relaxation is driven by bending, other options may be more viable. Using planar elements instead of beam elements adds further generality and reduces the number of overall assumptions. Many problems of elasticity can be satisfactorily represented by a 2-dimensional model. If one considers the silicon to be a planar geometry bonded to the elastomeric substrate, two situations can be modeled. A very slender ribbon of Si could be represented in two dimensions as a case of plane stress where the body is so narrow such that the stress along this dimension is assumed to be zero. These ribbons of Si are likely to be those first tested for the Si-PDMS anode system, thus it is desired to use Abaqus to model a plane stress Si thin film using CPS4R elements and a plane strain PDMS substrate using CPE4R elements. These two element types are linear elements with reduced integration to speed up processing time. They have two translational degrees of freedom per node and in structural analyses can support a third temperature degree of freedom (Abaqus Analysis User's Manual 2007). A rigorous study of these element choices along with demonstration of accuracy and FE model details is required.

2.5.1 Element Compatibility

The studies of the planar Si-PDMS anode system incorporates both plane stress and plane strain elements for the Si film and the PDMS substrate respectively. A series of patch tests (Lepi 1998; Irons and Ahmad 1980; MacNeal
1994; *NAFEMS A Finite Element Primer* 1992) are performed using both of these element types in a single simulation to determine their compatibility for the desired analysis. The details of the patch tests can be found in Appendix A and Appendix B. The test involves three stages: the first being a rigid body test, the second being a test that applies a state of known strain to the elements, and the final being a test to represent the desired loading by applying a thermal strain to the plane stress elements only. By studying the simulation results and comparing them to elastic theory (Boresi and Chong 2000), it is found that for the test performed the elements are compatible. In other words, they passed the tests by satisfying the equations from the theory of elasticity exactly. Therefore it is with confidence that the simulations proceed using the two different element types.

**2.5.2 Si-PDMS Convergence Study**

It is good practice to perform a mesh convergence study in order to be certain of the accuracy of the solutions of any analysis ("The Importance of Mesh Convergence" 2010). Such a study is performed on the planar simulation to determine an optimal mesh density for the system. The details of this study can be found in Appendix C. The geometry and mesh density of the optimal case (Case 3 from Appendix C) will be that of the analyses discussed in all subsequent sections.

**2.5.3 Stabilization**

The Si-PDMS anode system experiences local instabilities during the post-buckling. This is manifested by the appearance of a wavy structure in the Si material as it buckles under the developing compressive stresses. In order to
overcome convergence issues, stabilization is applied to the model at high strains. For instabilities, often times creative solution techniques (such as the arc length method or treating the simulation as a quasi-dynamic problem) may be required in order to obtain a converged result. Sometimes these techniques do not resolve any of the problems experienced with highly non-linear models or with local instabilities. Another technique well suited for tackling local instabilities is to use what is known as "stabilization." The details of how Abaqus implements stabilization can be found elsewhere (Appendix D). Fundamentally, stabilization incorporates viscous damping forces to aid in maintaining equilibrium when one part of the structure becomes unstable. This in essence adds artifacts to the model that must be minimized by the user. Refer to Appendix D for the discussion of the theory behind stabilization and all of the details regarding simulation results when stabilization is implemented on the Si-PDMS anode system. An optimal amount of stabilization to achieve a converged result at minimal artifact is found and implemented in all subsequent analyses.

2.6 Stress Relaxation

Using the Si-PDMS model that employs beam elements has established the proof of concept for using buckling as a means of stress relaxation. Now with the analysis criteria set for a more general, planar analysis in previous discussions (i.e. material properties, appropriate element choice, model dimensions, and stabilization parameters, etc.) a more rigorous and reliable study of the Si-PDMS anode system can begin.
The analysis procedure is identical to that detailed for the beam model; however the applied loads during the linear eigenvalue analysis must be altered (this was true for the mesh convergence and stabilization studies as well). The imperfection amount is confirmed to have no impact on the simulation results for stress and morphology (several imperfection amounts and mode shapes were tested and found to produce nearly identical results). During pre-processing the loads on the Si are changed from concentrated point loads at the left and right hand nodes to distributed compressive pressures along the left and right hand edges of the Si (Figure 2.10). The boundary conditions imparted to the PDMS remain the same; a bottom surface that is fixed. As before, the post-buckling is performed by implementing a small imperfection to a selected mode followed by the introduction of the thermal strain to the Si elements only.

Figure 2.10 A schematic demonstrating the boundary conditions and the applied loads for the linear buckling analysis of planar simulations

The thermal load applied to the nodes of the Si during post-buckling induces a strain in the elements of the material, laterally deforming the soft
substrate (Figure 2.11a). The CTE is the same for all elements of the Si material, thus with a uniform temperature applied, homogeneous diffusion is simulated for this particular analysis. Compressive stresses build within the Si due to the eventual constraint that the PDMS applies, and the Si remains flat until the critical strain of approximately 5% (Figure 2.11b-c). Similar to the previous analysis using beam elements, the amplitude of the waves continues to increase after buckling initiates and the waves will propagate down the length of the Si material with higher strain (Figure 2.11d-e).

Figure 2.11 Lateral deformation contour plots showing the evolution of the buckled morphology through the critical strain at (a) 3%, (b) 4.5%, (c) 5.5%, (d) 10%, (e) 15%, and (f) 20% strain (same scale).

The onset of buckling occurs after a critical strain of 5% and initially only a few waves develop at the center but then propagate with additional strain. The wavelengths and amplitudes are measured from the Abaqus model at several strains to qualify their trends (Figure 2.12). Since the Si material is only constrained by the substrate and is relatively free to expand, the wavelengths
settle at a constant value while the amplitudes increase linearly with higher applied strain. The deviations for this simulation are much lower than the previous one involving beam elements because the thin film has been meshed much finer down its length. This finer mesh produces more elements per wavelength than before, making dimensional measurements more accurate.

![Figure 2.12 Measured values, normalized by the Si thin-film thickness, for the buckled morphology of a planar simulation for (a) amplitude and (b) wavelength with ±2 standard deviation error bars.](image)

The equivalent stress (used as the failure criterion) for this planar analysis develops similarly to the previous simulation where the bending stress components dominate the stress state; containing a compressive, tensile and neutral zones through the thickness of the Si. The equivalent stress is driven primarily by the normal stress caused by bending, while the shear and the transverse stresses are nearly negligible. The plot of stress corroborates what the deformation contours have shown; a critical strain value of approximately 5% occurs just as buckling begins (Figure 2.13a). The behavior at higher strains is very similar to the previous analysis using beam elements; a dramatic increase in stress once buckling initiates followed by a linear stress-strain state dominated by
the bending associated with increasing amplitude. Again a stiff-substrate case is analyzed in order to quantify the amount of stress relaxation achieved, whereby it is evident that a large amount of lattice strain could be sustained before failure would occur by utilizing the stress relaxation of buckling (Figure 2.13b). Comparing the stress contour plots (Figure 2.14), one can observe that the magnitude of stress between stiff and soft substrate cases is greatly reduced and that buckling indeed does not occur before failure of the former case.

Figure 2.13 Stress of the Si showing the introduction of bending stresses at the critical strain of 5%: (a) the equivalent stress at the peak of the buckled waves and (b) the stress relaxation of the stress of the Si material for a soft (blue) substrate and for a stiff (red) substrate.

This planar analysis serves to verify the results from the proof of concept. It uses compatible elements with a converged mesh for accurate stress predictions. By incorporating soft materials into the design, buckling of the Si material will relax the induced stress caused by Li-ion diffusion by nearly an order of magnitude. The wavelengths are constant as the applied strain increases and the wave amplitude increases linearly, the primary cause for the increasing trend in the stress (i.e. the stress is driven by its bending component).
Figure 2.14 Comparison of the stress contour plots of the Si thin film bonded to a stiff and soft substrate at the same scale

2.7 A Three-Dimensional Simulation

A three-dimensional model of the Si-PDMS system would provide the means to account for lithiation (or lattice expansion) in all three directions of the Si lattice. Additionally, performing a 3-D analysis will further generalize the model and limit the assumptions. Abaqus is again used to perform a preliminary finite element analysis. The Si is represented as a ribbon that is 300µm long, 2µm wide, and 100nm thick. The PDMS must be made thick enough and wide enough such that the effects of the boundary condition applied to the base and the edge effects will not propagate to the Si ribbon. The goal of this simulation is to briefly investigate the behavior of this general model when the Si ribbon is subjected to an applied thermal strain (i.e. Li-ion diffusion). This analysis will qualitatively study a general three-dimensional case of the Si-PDS anode system.
In order to improve solution processing time, the entire Si-PDMS system is divided in half along a plane of symmetry (Figure 2.15). This technique reduces the amount of elements required to analyze large models. 3D brick elements (C3D8R) are used for the Si ribbon and a combination of brick and tetrahedral elements are used within the PDMS (Figure 2.16). The ribbon is discretized such that its element aspect ratios are close to those previously determined; however only two elements are created through the ribbon's thickness. While it is not ideal to have just two elements through the thickness, the difficulty of meshing such a thin structure bonded to a very thick structure is compounded when adding the third dimension. The analysis procedure is similar to that of the two dimensional methodology: the base of the PDMS is fixed in all six degrees of freedom for all numerical studies, the Si and the PDMS are bonded together at their coincident nodes using a tie constraint, a linear eigenvalue buckling analysis is performed, and a nonlinear post-buckling simulation is performed on a model that incorporates a 1% imperfection of the designate mode from the linear analysis. The post-buckling again is intended to simulate the Li-ion insertion, such that the thermal strain is applied to just the elements of the Si ribbon.

For the 3D analysis, a critical strain is calculated to be approximately 1.5%. This is significantly less than previous results, and is attributed to the complexity of the triaxial stress state of the Si ribbon. In the same fashion as the previous analyses, the Si material expands until it is restricted by the substrate (Figure 2.17a). The increasing compressive stress cause the structure to turn
Figure 2.15 A schematic of the 3D analysis performed on the Si-PDMS anode system where the symmetry is utilized by modeling only half of the entire structure (the right hand side)

Figure 2.16 The meshing used for the 3D analysis: (a) the substrate is finely meshed near the Si-PDMS interface and (b) the meshing strategy for the Si ribbon and the neighboring PDMS

unstable and buckling occurs (Figure 2.17b). The amplitude of the wavy buckled shape increases with increasing applied strain (Figure 2.17c-e). The trends of amplitude (Figure 2.18a) and wavelength (Figure 2.18b) are consistent with previous analyses. After buckling has occurred the amplitude increases
dramatically but then increases linearly with respect to the applied strain and the wavelength remains relatively constant.

Figure 2.17 Lateral deformation contour plots showing the evolution of the buckled morphology through the critical strain at (a) 1%, (b) 2%, (c) 3%, (d) 4%, (e) 4.5%, and (f) 5% strain (same scale).

The development of stress within the Si ribbon is consistent with previous analyses (Figure 2.19). After the critical strain the bending stress (here the stress that is along the ribbon's length, the axial direction) dominates the stress state just...
like the two-dimensional simulations. If this trend were to continue, the analysis would predict a failure of 2.6 GPa occurring at approximately 26% strain. Thus the stress relaxation is realized in three-dimensions as well. The maximum strain achieved for this simulation was 5% strain because further progression required too small of time increments that were simply too computationally expensive.

Further study of a three dimensional model would require significant computational resources. Challenges exist with the three dimensional model and include the immense computation effort required, the expansion of the Si ribbon along its width could cause a twisting effect under the applied thermal strain, and the required mesh density of the substrate near the interface is tremendous. Stabilization was not employed for this analysis because an appropriate level was unknown and test of several values was cost-prohibitive. Suggestions for further study would include determining the effects of the Si ribbon width and determining the optimal dimensions for the substrate in order to remove excess material thereby reducing the overall system weight.
Figure 2.19 Plot of the stress within the Si ribbon demonstrating the introduction of bending stresses at the critical strain of 1.5% and a linear relationship with the applied strain after buckling initiates

2.8 Summary

Several models have been created in order to test the hypothesis that a silicon anode bonded to a compliant substrate will indeed relax the stress caused by Li-ion insertion. It has been shown with the rigorously examined planar model that a thin Si material, when only constrained by its substrate, will buckle due to the applied strain at a relatively constant wavelength and increasing amplitude. This buckling relieves the stress by an order of magnitude when compared to a Si anode bonded to a very stiff substrate where no buckling occurs. This stress relief has tremendous implications for Li-ion batteries. By utilizing the buckled Si material with compliant substrates, the number of cycles to failure will increase because the stress state will be significantly lower than a conventional battery cell design. Thus in preserving the Si material from pulverization, the performance of a Li-ion battery that incorporates soft materials and allows for this buckling will be enhanced greatly. Example input files for both the planar and the three-dimensional analyses created using Matlab can be found later in this document.
(Appendix E and Appendix F). While these are not fully autonomous, as the user will be required to input node and element creation script lines (usually from Abaqus CAE input file generation) for irregular meshes, these examples serve as a foundation to performing these analyses in this thesis.
CHAPTER 3
THE EFFECTS OF NON-UNIFORM LITHIUM CONCENTRATION ON
SILICON ANODE STRESS RELAXATION

3.1 Introduction

The analyses thus far have studied how the morphology and stress evolves within an elastic thin film Si anode. By utilizing soft substrates a significant amount of deformation can be accommodated and the stress induced by Li-ion diffusion is relaxed. These results, however, come from models where the simulated diffusion is homogeneously distributed to the entire Si film. In other words, each element of Si, all with the same CTE, experience equivalent thermal strains with the applied temperature load. Therefore the only constraint to the ensuing expansion is the soft, PDMS substrate. This homogeneous diffusion may be the ideal case because all parts of the Si film are contributing equally to the operation of the anode. It is reasonable to conclude that homogeneous diffusion into the solid Si material can be achieved by using anodes with sufficiently short diffusion lengths (i.e. thin nanostructures) or by charging the anode slowly such that there is sufficient time for the Li-ions to transport from the surface to the base of the anode. The actual parameters that define and relate things such as charge rate, Li-ion concentration, diffusion induced strain, etc. for this type of anode system are unclear at the present time, thus the simulations discussed in this chapter serve to qualitatively study the effects of different charge rates which would produce a gradient of Li concentration through the Si thickness. The goal
of these analyses is to determine trends from which useful information can be obtained for application to experimental and further numerical work.

3.2 Analysis Procedure

For this investigation, the Si material is again represented by plane stress elements while the substrate is made up of plane strain elements. The analysis procedure is identical to the methodology established for the planar simulation in Chapter 2. As before, the post-buckling is performed by implementing a small imperfection to a selected mode followed by the introduction of the thermal strain to the Si elements only. The difference from previous analyses is that the applied lithiation strain now varies through the thickness of the Si anode. By introducing a thermal strain to the Si material that is greater at its exposed surface than at the interface with the PDMS represents a lattice that is being strained more heavily at the surface due to a greater degree of Li-ion diffusion. The extent of this depends upon the rate of charging. In other words a faster charge rate causes a larger gradient of strain through the thickness than a slow charge rate which causes a more uniform strain to occur within the Si material.

The Si film is that of a linear elastic material with a specified Young's modulus and Poisson's ratio. The thermal expansion is determined by the specified CTE. Recall that the Si thin film is meshed with four elements through its thickness. Thinking of each row of elements as a layer (Figure 3.1), a variable thermal strain can be created by either applying a constant temperature to all four layers and assigning different CTEs to each layer or by applying a varying temperature to each layer and assigning the same CTE to all the layers. For this
study of the effects of charge rate, the former case is employed; however both approaches would be appropriate. Either approach will create the same thermal strain, which is the "real" quantity for the analogy between lithiation-thermal strain; however the latter approach may be subject to smaller numerical errors. The layers are created by partitioning the 100nm thin Si film into four parts which are assigned different sections to which different material properties can be easily assigned within the analysis input/script files. Each layer has one element through its thickness for a total of four through the entire film thickness. No bonding is required between the Si layers as the nodes between two layers are shared because the partitioning serves to create a separate section within a single part, not separate parts of themselves. The analysis itself is a static analysis, not a transient one. Thus the rate effect is interpreted as such: for each increment of the applied temperature to simulate diffusion, a certain (unknown) amount time has passed, and during this time period each layer experiences a different amount of simulated diffusion-induced strain. Therefore during a given increment in the load step (time), a varying level of strain is experienced in each layer, representative of a varying degree of diffusion.

As previously stated, the charge rate effect is simulated by applying a consistent temperature to all the nodes of the Si while assigning variable CTEs to each layer. Four cases are investigated (Table 3.1) whereby the top layer, Layer 1, of the Si material is assigned the bulk CTE value of Si, 2.6·10^{-6} °C^{-1} (Tokumaru and Okada 1984) and the bottom layer, Layer 4, is assigned with 100%, 90%, 80%, and 70% of this bulk value. The choice of the CTE is arbitrary and so is the
applied temperature to obtain a desired thermal strain because the quantity of interest is the product of the two, the thermal strain. The CTEs of the two intermediate layers are calculated by linearly interpolating between the values of the top and bottom layers. Note that the first case of 100% has already been performed, as it represents the homogeneous diffusion of Li-ions into the Si that has been discussed in Chapter 2. A model that incorporated six layers (using the same Si aspect ratio reported from the mesh convergence study) was created, but it showed no significant improvements from the four layer model, thus it was not scrutinized based upon the grounds of computational efficiency.

It is predicted that fast charge rates will result in less than desirable performance. Mechanically, the bottom layer(s) of the Si material located at the Si-PDMS interface will not expand to the extent of the top layers at the free surface. This mismatch in deformation induces mechanical strains that are much
Table 3.1

Charge Rate Effect Analysis: Coefficient of Thermal Expansion Assignments

<table>
<thead>
<tr>
<th></th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
<th>Case 4</th>
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</thead>
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<td>90% Bulk</td>
<td>80% Bulk</td>
<td>70% Bulk</td>
</tr>
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</tr>
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<td>2.43·10⁻⁶</td>
<td>2.25·10⁻⁶</td>
<td>2.08·10⁻⁶</td>
</tr>
<tr>
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<td>2.60·10⁻⁶</td>
<td>2.34·10⁻⁶</td>
<td>2.08·10⁻⁶</td>
<td>1.82·10⁻⁶</td>
</tr>
</tbody>
</table>

greater than those that exist if the lithiation strain is uniform. This increase in strain would cause significant stresses to develop in the stiff Si material. Thus the bottom layers would in essence serve somewhat as substrates to the top layers.

3.3 The Effects of Charge Rate

The primary variable of interest here is the evolution of the stress within the Si material. Thus for each load case, the maximum equivalent stress in the Si material is obtained from the FE results for comparison. The location of this maximum stress is in Layer 1 at the center-most wave for the cases where buckling occurred. Each case is compared using plots of stress versus the applied strain (Figure 3.2). The strain on the horizontal axes is that calculated for the top layer (i.e. the product of the incremental temperature and the bulk material's CTE) in order to readily compare it to the homogeneous diffusion case.

It can be seen that before the critical buckling strain the slope of the stress-strain relationship increases with faster charge rate. This is attributed to the influence of the bottom layers of the Si experiencing less thermal expansion, subsequently acting as a substrate to the top layers. Just as seen before, once buckling is initiated, the stress state becomes dominated by the bending
component and there is further increase in the stress. Subsequently the stress behaves rather linearly with respect to the applied strain attributed to the increasing amplitude of the waves. The fourth case did not show signs of buckling occurring before the solution began to diverge. The solutions for the latter three cases failed to converge at some point during the load step up to 25% strain, after which the stress is estimated based upon the trends before the solution stopped and upon experience from previous simulations.

It was observed that the critical strain to cause buckling increases with faster charge rate (Table 3.2). This is a disadvantage of charging at higher rates because of the stress relief caused by buckling coupled with the smaller slope before buckling initiates. By using homogeneous diffusion, the applied strain to cause failure (i.e. stress in excess of 2,600 MPa) is improved two-fold or more when compared to the other cases simulated.

![Figure 3.2 Plots of stress comparing the four charge rate test cases (dashed lines represent the expected trends of the simulations).](image-url)

Figure 3.2 Plots of stress comparing the four charge rate test cases (dashed lines represent the expected trends of the simulations).
Table 3.2

Charge Rate Effect Results: Comparison of the critical & failure strains

<table>
<thead>
<tr>
<th></th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
<th>Case 4</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>100%</td>
<td>90%</td>
<td>80%</td>
<td>70%</td>
</tr>
<tr>
<td>Critical Strain [%]</td>
<td>5.0</td>
<td>5.6</td>
<td>6.1</td>
<td>N/A</td>
</tr>
<tr>
<td>Strain at Failure [%]</td>
<td>30</td>
<td>14.8</td>
<td>9.1</td>
<td>8.9*</td>
</tr>
<tr>
<td>Failure Strain Difference [%] (Compared to Case 1)</td>
<td>N/A</td>
<td>50.7</td>
<td>69.7</td>
<td>70.3</td>
</tr>
<tr>
<td>Predicted Stress at 25% strain [MPa]</td>
<td>1,900</td>
<td>4,000</td>
<td>5,900</td>
<td>7,300</td>
</tr>
</tbody>
</table>

*This value is predicted based upon expected trends

3.4 Summary

The results from the charge rate simulations verified the original conjecture that homogeneous diffusion is highly desired. This is because uniform diffusion takes advantage of both the compliant substrate permitting extensive deformation and the stress relief caused by buckling. This begs the question as to how to ensure that this will occur. A thin film anode, due to its short diffusion length, is much more likely to experience uniform diffusion as opposed to a thick one or a bulk material. Truly, the diffusion of Li in Si would take only a fraction of a second in Si thin films (Sethuraman et al 2010; Yoshimura et al 2007), thus the homogeneous diffusion case is quite plausible for the Si-PDMS anode system. This will allow full advantage to be taken from the stress relaxation that occurs by using buckling and soft substrates. Bulk silicon will therefore not benefit from the stress relaxation from soft substrates due to the non-uniform Li concentration. Apart from the stress relaxation, the homogeneous diffusion argument is another aspect of the Si thin film anode that is so attractive; that diffusion occurs through the entire thickness using the majority of the Si for the electrochemical reaction.
CHAPTER 4

THE EFFECTS SILICON THIN FILM PLASTICITY

4.1 Introduction

Studies regarding plasticity of thin films range between many different approaches, techniques, and produce a variety of outcomes. Most often researchers utilize nanoindentation in order to ascertain the material properties of a thin film. Several studies can be found that investigate the response of thin metallic films such as copper (Xiang and Vlassak 2006; Dehm and Arzt 2000), aluminum, titanium (Bahr et al 2003), gold (Espinosa and Porok 2001; Lacour et al 2003; Salvadori et al 2003), platinum (Salvadori et al 2003), etc. to various stimuli. The type of substrate used ranges from soft, elastomeric substrates (Bowden et al 1998; Huck et al 1999; Huang and Suo 2002; Jiang et al 2007; Zhao et al, 2007) to stiffer silicon or metallic substrates (Dehm and Arzt 2000; Saha and Nix 2001; Zhang et al 2007) and many researchers have used a combination of soft-film-stiff-substrate or stiff-film-soft-substrate. Fewer have studied in detail the effects that a material's inelastic or plastic behavior can have, sometimes only going as far as to attribute fracture or failure of the thin film to plastic deformation (Bahr et al 2003). Fewer still are articles involving buckling of thin films and the resulting plastic behavior. Plastic folding of gold films bonded to silicon substrates has been studied as a form of blistering (Colin et al 2007), and some failure modes within hard films of TiN have been observed as buckling or spalling, attributed to plastic deformation and elastic recovery (Bull 1997).
A very recent study regarding the in situ measurements of stress within Si thin films used as anodes for Li-ion batteries have only begun to shed light on how the stress develops due to lithiation (Sethuraman et al 2010). The article highlights observations of plastic flow leading to strain hardening within the Si electrode (whereby the stress is calculated by monitoring the curvature of the electrochemical cell and using the Stoney equation) in order to accommodate the immense volumetric expansion that occurs. The authors infer an initial elastic response where the stress evolves linearly with cell capacity until the compressive stress of the film causes yielding and it begins to flow with continued lithiation. With regard to the elastoplastic nature of Si thin films on elastomeric substrates, no published work has been found despite exhaustive efforts by the author. Thus it is the intention of this study to perform some qualitative analysis on the effects of plasticity for Si anodes bonded to compliant substrates. Due to the lack of experimental data, the liberty to choose plastic properties of Si has been taken in order to facilitate this qualitative investigation.

4.2 Plasticity and Abaqus

Abaqus adheres to the incremental plasticity theory in order to carry out elastic-plastic numerical calculations. The fundamental assumption is that the deformation can be divided into an elastic and an inelastic (plastic) component according to the strain decomposition of

\[ \mathbf{\varepsilon} = \mathbf{\varepsilon}^e + \mathbf{\varepsilon}^p \]  \hspace{1cm} (4.1)
where $d \varepsilon$, $d \varepsilon^e$, and $d \varepsilon^p$ are the total, the elastic, and the plastic strain increments respectively (Chen and Han 1988). According to von Mises yielding criterion the yield condition, $k$, (determined by performing uniaxial tension tests) is

$$k = \sqrt{2} \sigma_o$$  \hspace{1cm} (4.2)

where $\sigma_o$ is the yield limit from the uniaxial stress-strain curve (Hinton 1992).

Generalizing the elastic limit requires a yield function, $f(\sigma_{ij})$,

$$f(\sigma_{ij}) = F(\sigma_{ij}) - k$$  \hspace{1cm} (4.3)

and the location where the material behavior changes from elastic to plastic is called the yield surface

$$F(\sigma_{ij}) = k$$

Thus a plastic response for rate independent materials (Abaqus Theory Manual 2007) occurs when

$$f(\sigma_{ij}) = 0$$

The associated flow rule is postulated for plastic flows in order to define the direction of the plastic strain components and to determine their relative magnitudes as

$$d \varepsilon^p_{ij} = d \lambda \frac{\partial f}{\partial \sigma_{ij}}$$  \hspace{1cm} (4.4)

where $d \lambda$ is a scalar of proportionality (Chen and Han 1988). Abaqus uses the associated flow rule for rate independent elastoplastic materials. According to the
flow rule, the plastic flow "moves" along a path normal to the yield surface (Chen and Han 1988).

After the initial yield, Abaqus utilizes increments in strain to determine if the material continues to flow plastically. According to von Mises criterion, the incremental effective plastic strain (a scalar quantity) for strain hardening materials is calculated according to

\[
de_{eff}^p = \sqrt[3]{\frac{2}{3} \delta \epsilon_{ij} \epsilon_{ij}^{pl}}
\]

(4.5)

and the subsequent yield condition is given as

\[
F^2 = \frac{1}{2} s_{ij} s_{ij} - 3 \sigma_o^2 e_{eff}^p = 0
\]

(4.6)

where \( s_{ij} \) is the deviatoric stress component (Hinton 1992). The effective stress, \( q \), is calculated according to

\[
q = \sqrt[3]{\frac{3}{2} s_{ij} s_{ij}}
\]

(4.7)

(Chen and Han 1988; Abaqus Theory Manual 2007). Within the software, the strain is incremented and the effective stress is evaluated based upon a purely elastic response (Abaqus Theory Manual 2007). If the calculated stress violates the yield condition then the software must iterate the stress increment (with trial values for the stress) using the backward Euler method to the scalar constant, \( \lambda \), around the trial stress state (Hinton 1992; Abaqus Theory Manual 2007). The new stress and plastic strains can be calculated after \( \lambda \) is known. Iterations continue until the yield condition is satisfied. In depth details of the backward Euler method as applied to numerical plasticity analysis can be found in Appendix.
G and elsewhere (Hinton 1992). For a plane stress material, the out-of-plane stress component is zero and the out-of-plane strain component is predicted by

\[
\hat{\varepsilon}_{zz} = -\frac{V}{1-V}\left(\varepsilon_{xx}^{ei}\left|_{t} + \Delta\varepsilon_{xx} + \varepsilon_{yy}^{ei}\left|_{t} + \Delta\varepsilon_{yy}\right)\right)
\]

(4.8)

where \(\varepsilon_{xx}|_{t}\) and \(\varepsilon_{yy}|_{t}\) are the elastic strain components calculated from the test stress quantities and the \(\Delta\varepsilon_{xx}\) and \(\Delta\varepsilon_{yy}\) are the total increments in strain (Abaqus Theory Manual 2007). The plane stress condition will be satisfied once the correct plastic straining is obtained (Abaqus Theory Manual 2007).

4.3 Analysis Procedure

The plasticity of the Si anode is not fully understood at this time; therefore this work attempts to qualitatively examine the results of a sample elastoplastic behavior. The work by Sethuraman et al. suggests that a strain hardening material would be appropriate for this qualitative study (2010). Therefore a bi-linear material model is implemented for the Si within the planar Abaqus model (Figure 4.1) with an elastic modulus, \(E\), and a tangent modulus, \(E^{t}\), for the behavior beyond yielding.

![Figure 4.1 The stress-strain material relationship model for a material at current stress state \(\sigma\) at a given total strain \(\varepsilon\).](image-url)

\[
\Delta\sigma = \sigma - E\varepsilon_{0} \\
\sigma = E\varepsilon_{0} + E^{t}\Delta\varepsilon
\]
Using an incremental definition for the deformation, the strain increments can be defined individually as

\[ d\varepsilon = E^t d\varepsilon \]  \hspace{1cm} (4.9)

\[ \varepsilon d\sigma = E^p d\varepsilon^p \]  \hspace{1cm} (4.10)

\[ d\sigma = E d\varepsilon^e \]  \hspace{1cm} (4.11)

where \( E^t, E^p, \) and \( E \) are the tangent, plastic, and elastic moduli respectively (Chen and Han 1988). Letting the tangent modulus be some fraction of the elastic modulus such that

\[ E^t = \eta E \]  \hspace{1cm} (4.12)

where \( 1 > \eta > 0 \), and substitution of equation (4.9) through equation (4.12) into equation (4.1) gives an expression for the plastic modulus as

\[ E^p = \frac{\eta}{1-\eta} E \]  \hspace{1cm} (4.13)

Abaqus can support user-input data for the stress-plastic strain relationship; however the stress input is the instantaneous yield stress as a function of the plastic strain,

\[ E^p = \frac{dY}{d\varepsilon^p} \]  \hspace{1cm} (4.14)

where \( dY \) is the incremental change in the current yield stress, \( Y \). Thus an arbitrary relationship can be created and studied. The user must input two columns of data: the yield stress and the corresponding plastic strain. For the bi-
linear elastoplastic material, the yield stress is incremented by any amount and the corresponding plastic strain increment is calculated according to equation (4.14) by dividing the yield stress with the known plastic modulus.

A yield stress is assumed to be 130 MPa, after which the material modulus decreases according to equation (4.12) and equation (4.13). The value of $\eta$ used is $1/10$. This material model is placed within the Abaqus simulation as a stress dependent upon plastic strain according to flow theory. The PDMS substrate is assumed to be completely elastic for this analysis. Again the Si material is represented by plane stress elements while the soft substrate is composed of plane strain elements. The analysis procedure is identical to the methodology established for the planar simulations in Chapter 2. As before, the post-buckling is performed by implementing a small imperfection to a selected mode followed by the introduction of the thermal strain to the Si elements only. This will deform the Si film beyond its elastic limit where the plastic behavior causes some intriguing changes to the Si morphology. These changes in the morphology have striking ramifications on the evolution of the stress within the self-assembling buckled Si film.

4.4 The Effects of Plasticity

The deformation of the Si material reveals an interesting effect when plasticity is introduced into the model. At approximately 5.5% thermal strain, the first of the Si elements enter the plastic region of their equivalent stress-strain relationship. According to Huck et al (2000) and Jiang et al (2007) the
wavelength of buckled Si bonded to a soft substrate is related to the ratio of the film modulus to the substrate modulus according to

\[ \lambda \propto \left( \frac{E_f}{E_s} \right)^{\frac{1}{3}} \]  

(4.15)

Once a portion of the Si material experiences a stress greater than the yield stress, the Si modulus is reduced causing a drastic change in wavelength to occur. This is due to the aforementioned relationship between the wavelength and the ratio of the moduli, \( E_f \) and \( E_s \). The wavelength will begin to develop as it had in the linear elastic case (critical buckling strain of approximately 5% with initially shallow waves), however once buckling begins the stress rises very quickly above the yield stress due to the introduction of a bending component, and a change in the average wavelength is observed (Figure 4.2b). The waves’ amplitude is also affected by the transition from elastic to plastic (Figure 4.2a). The average amplitude is initially very shallow, however it increases rapidly at the onset of buckling, but once the elements of the Si material begin to turn plastic this behavior curbs. As the waves change in wavelength, the amplitude of the resulting wavy structure is characterized by a very gradual increase in magnitude. The greatest deviation occurs near the local transition from elastic to plastic. This is caused by the abrupt change in morphology making dimensional measurements more difficult. Included with this thesis are 3 videos (Stress.avi, PEEQ.avi, and Def.avi) that detail the evolution of the deformation, stress, and plastic strain of the Si anode system as the applied strain is induced in the Si material (Appendix
These videos help to understand how the change in morphology affects the resulting stress state in the Si thin film.

Figure 4.2 Normalized measurements for the elastoplastic model: (a) a gradual increase in the average amplitude and (b) a significant drop in wavelength as the material turns plastic.

Figure 4.2 Normalized measurements for the elastoplastic model: (a) a gradual increase in the average amplitude and (b) a significant drop in wavelength as the material turns plastic.

Studying the plot of wavelength, it is apparent that a drastic change in the morphology of the Si material occurs once the elements begin to enter the plastic region. The resulting waveform is symmetric about the centerline of the model, and the center is a critical location where buckling occurs first. It is at this center location where the elements first exceed the specified yield stress, resulting in the change in wavelength first occurring at the film center. The stress of the center elements is recorded and several zones can be identified (Figure 4.3). At the onset of buckling the stress is below the yield stress (Figure 4.3a) and the observed waveform consists of shallow waves (Figure 4.5a). The plastic strain, or the equivalent plastic strain, calculated according to equation (4.5) is observed to be zero during this zone (Figure 4.4a). The stress increases dramatically because of the bending stress that develops during buckling coupled with the transition from elastic to plastic (Figure 4.3b and Figure 4.4b), causing the wavelength to
shorten in a localized region (Figure 4.5b). This shift in wavelength causes significantly more bending to occur. The wave at the center is then unloaded (Figure 4.3c and Figure 4.4c) due to the formation of neighboring waves that are simultaneously experiencing a rapid transition from elastic to plastic (Figure 4.5c). The formation of these short wavelengths propagates down the length of the Si-PDMS system as the applied strain increases and more elements enter the plastic region. The local wave is then reloaded as a result of the increase in amplitude (Figure 4.3d and Figure 4.4d). Once the stress state that was obtained before unloading began is once again reached, the transition in slope of the stress curve (Figure 4.3e) is evidence that the plastic deformation begins to flow again (Figure 4.4e). As the waves propagate and the amplitude of the existing waves increases, the bending stress (i.e. the normal stress on the thin film cross-section) continues to dominate the stress state.

Figure 4.3 Plot of equivalent stress within the Si showing (a) the initiation of buckling at approximately 5% strain, (b) the high degree of stress caused by localized wavelength shift, (c) the local unloading due to the formation of short wavelength buckles near the centermost buckle, (d) the subsequent reloading of the local wave, and (e) the increase in stress according to the specified plastic modulus caused by resumed plastic straining.
Figure 4.4 Plot of the equivalent plastic strain (PEEQ) at the center of the Si material showing (a) the start of plastic straining shortly after buckling begins as approximately 5% strain, (b) the dramatic increase in the plastic strain due to the sharp wavelength shift, (c) the local unloading causing no increase in plastic strain, (d) and the subsequent reloading of the local wave causing an elastic response until (e) the increase in plastic strain continues once the stress level before unloading is reached again.

Figure 4.5 The morphology as (a) buckles appear within the Si anode material at 5% strain, (b) local buckles occur where plasticity begins at approximately 5.5% strain, (c) new waves propagate stretching the existing waves between 6% and 8% strain, and (d) the wave propagation continues down the length of the Si anode material at strains above 6% strain (same scale).

Once again a stiff substrate simulation is performed as a benchmark that uses the elastic-plastic material model for the thin film only. The results are consistent with previous tests, whereby the buckling will relieve the stress by
nearly an order of magnitude at the high strains (Figure 4.6). The stress contour plots (Figure 4.7) show that the magnitude of stress between soft and stiff substrate cases is greatly different and that the thin film will not buckle when attached to a stiff substrate before it fails.

Figure 4.6 Plots of the equivalent stress within the Si material showing a comparison of the soft and stiff substrate for the case of a plastic Si anode material.

The stress evolution within the Si material can be viewed from a second point of view. At high strains, once the new wave morphology has developed for a significant portion of the thin film (Figure 4.5d), the magnitude of the stress of each peak is nearly identical. Averaging the stress between several waves at each increment of applied thermal strain yields a very smooth plot of stress that doesn't have the unloading features previously explained (Figure 4.8a). While this plot does not detail the dramatic morphology change, it accurately details the average stress within the Si material during the lithiation process. At the high, 25% strain the equivalent stress is approximately 500MPa similar to previous results for a single wave at the film's center (Figure 4.3) showing nearly an order of magnitude
Figure 4.7 Equivalent stress contour plots of the elastoplastic Si material demonstrating the stress relaxation (the legend is consistent for both contour plots)

difference when compared to the benchmark, stiff substrate case (Figure 4.8b). This plot serves as a simple demonstration that the stress is impacted by the incorporation of a plastic material model, however it is still relieved due to the buckling.

4.5 Summary
Qualitatively studying the strain hardening behavior of plasticity has produced very interesting results. After the critical strain occurs and buckling begins the stress within the Si material rises quickly due to the bending component. Upon exceeding the yield stress, a change in the material modulus necessitates a change in the morphology (wavelength and amplitude). Thus the bending component of stress increases drastically to accommodate the change in morphology. The change in modulus has an obvious effect on the morphology of the Si and also promotes further stress relaxation due to the reduction in material modulus. Thus
one could predict that any change in the material's constitutive behavior will have subsequent ramifications on the morphology. In other words, the buckling occurs at 5% strain due to an instability that initiates buckling and a change in the Si material modulus will add further instability as the structure will require a change in the buckled morphology to relieve its strain energy. In order to validate this, in situ experimental observations are required to determine the extent of morphology change.
5.1 Introduction

The promising results from the finite element simulations have triggered endeavors into performing experiments in order to further validate the claim on stress relaxation within Si anodes. These preliminary experiments are being performed by colleagues as a first look into the practicality Si-PDMS anode system. The results of these experiments are quite exciting; indicating long cyclic stability due to the development of a wrinkled Si structure. In support of the analysis work discussed in this thesis the results from the tests that have been completed so far are presented here very briefly as a summary of a paper that is in preparation (Yu et al. 2011) in support of the analysis work performed for this thesis. My contribution to the aforementioned paper was that of the numerical FE simulations, which demonstrated the concept of stress relaxation.

5.2 Experimental Results

A sample battery cell that incorporates a Si-PDMS anode (Figure 5.1) is fabricated in an argon-filled glovebox starting with wide Si ribbons (approximately 50-80 μm wide and 70-350 nm thick) etched from silicon-on-insulator (SOI) wafers. After the etching, the Si ribbons rest on the insulating SiO$_2$ material. Layers of gold (Au) and chromium (Cr) are applied to the Si ribbons to serve as the current collector and as a bonding agent to the elastomeric substrate respectively. PDMS (1 to 3 mm thick) to be used as the substrate is brought into
conformal contact with the multilayer, Au-Cr-Si, structure. The PDMS is peeled away to form the completed Si-PDMS anode system. As a means of wiring out, a layer of Au and Cr are deposited at the ends of the ribbons. The cathode is a Li metal foil, used as a counter electrode and a reference, and the electrolyte used is 1 M LiPF$_6$ + EC + DEC (1:1 in volume). A conductive polymer (polypropylene / polyethylene / polypropylene) coats both electrodes and acts as a separator. Thus a complete cell is created for testing purposes. The Si-PDMS anode system (Figure 5.2a) is placed within the test cell along with the other components (Figure 5.2b) which is prepped for testing.

![Schematic of the fabrication process of Si anodes on PDMS substrates](image)

Figure 5.1 Schematic of the fabrication process of Si anodes on PDMS substrates
Electrochemical testing is conducted and afterwards the Si anodes are observed to buckle. The entire cell demonstrates stable energy capacities to 500 cycles. It is believed that the capacity retention is directly related to the anodes remaining intact and maintaining good contact during the long life cycle. A wavy morphology in the Si ribbons is seen as early as the first cycle (Yu 2010), verifying the hypothesis that the lithiation strain cause the Si thin films to buckle. Optical and SEM images (Figure 5.3) of the Si anode after several cycles indicate a mixture of smooth, one-dimensional wavy structures and very complex, labyrinthine structures. The former geometry is the expected result based upon the finite element analysis. The latter geometry is believed to be a possible result of a ribbon initially with a two-dimensional wavy shape or a herringbone pattern caused by increasing amounts of compressive lithiation strains. The morphology
changes are likely due to a nonuniform state of charge caused by nonuniform contact with the current collectors in combination with the plasticity of the Si film during lithiation. This result is fascinating and warrants further investigation.

Figure 5.3 Optical microscope and SEM images of (a) smooth buckled Si ribbon and (b) herringbone patterns, and (c) labyrinthine wrinkles.

The excellent cyclic stability of the test cell up to 500 cycles shows only a loss of 15% specific capacity, an extremely low average fading rate of 0.03% per cycle (Figure 5.4a). The discharging capacity is measured to be approximately 3,500 mAh/g at 500 cycles. This data indicates that the Si-PDMS anode system provides a much improved overall cycling stability and performance compared to other Si electrodes, which usually fade quickly after several tens of cycles due to the volumetric expansion and contraction during Li ion insertion and removal. For example, a conventional graphite anode has a discharge capacity of about 800 mAh/g (Kasavajjula, Chunseng, and Appleby 2007), 1,170 mAh/g during the first discharge for bulk Si (Ryu et al 2004), 300 mAh/g for amorphous Si anodes (Bourderau, Brousse, and Schliech 1999), approximately 1,000 mAh/g for Si/graphite anodes and Si coated composites (Holzapfel et al 2005; Liu et al
2005a), 600 mAh/g for Si with elastomeric binders (Liu et al. 2005b), and approximately 3,000 mAh/g for Si nanowire anodes after 10 cycles (Chan et al. 2008). The high-performance and superior stability is primarily due to the unique combination of the intrinsically high-capacity Si and the PDMS which helps to release the stress via buckling of the Si ribbons. The buckled morphology reduces the accumulation of stress to avoid fracture, behaving like a cushion, contributing to preserve the Si material for a long cyclic life-span. The Si-PDMS anode system has a very high Coulombic efficiency (the ratio of the current discharge capacity compared with the previous discharge capacity), averaging between 99.5% and 100% during the entire 500 test cycles (Figure 5.4b). This data supports the conclusions regarding the reduced capacity fading, demonstrating that the PDMS substrate plays a crucial role in allowing the expansion and contraction of the Si anode throughout many cycles. The charge-discharge profile for the test cell also serves to demonstrate the outstanding stability of this dynamic process of Li insertion/removal from the Si lattice (Figure 5.4 inset).

![Figure 5.4](image)

Figure 5.4 (a) Cyclic stability of the battery cell up to the 500th cycle with nearly 85% capacity retention. Inset: Typical charge/discharge profiles and (b) Coulombic efficiency from the 1st to 500th cycle showing 99% to nearly 100% efficiency. Inset: Charge/discharge profiles of several cycles.
5.3 Summary

The results of the experiments have been summarized briefly in this chapter. They are very exciting, verifying that buckling does indeed occur upon lithiation, after which the buckled shape acts like a spring to accommodate the large strains caused by cyclic Li insertion and removal. Because of this unique characteristic, a long cyclic stability due to the development of the wrinkled Si structure is evidenced during electrochemical testing. The wrinkled morphology appears to be able to take on a variety of forms, the cause of which is uncertain of at this time. These experiments serve to confirm the original hypothesis that a flat Si bonded to an elastomeric material will indeed buckle due to the diffusion-induced compressive stressed. This buckling serves to relax the stress during the cycles of battery operation. A very high cyclic stability is obtained using the Si anodes on soft substrates, with a discharge capacity of 3,500 mAh/g. It is believed that further work to understand the mechanism behind the stress relaxation along with efforts to optimize cyclic performance will bring about new designs that can realize capacities closer to the theoretical maximum.
CHAPTER 6
SUMMARY AND CONCLUSIONS

6.1 Summary of Finite Element Analysis and Experiments

Early attempts at utilizing Si in Li and Li-ion batteries because of its highest known energy capacity have shown early capacity fading and limited cycles before failure due to the difficulties resulting from large volume expansions which cause the Si material to self-pulverize. Using composite materials or nanostructures have typically avoided this issue to obtain better cyclic stability at a cost of overall effectiveness or practicality. Thus a means of relaxing the stress to utilize Si at its fullest potential while obtaining high cyclic performance is the major goal. In order to test the concept of stress relaxation in Si anodes for Li-ion batteries, finite element analyses were conducted on a straightforward model. The results from these simulations indeed show that a Si film on a compliant substrate experiences stress relief when compared to a similar system with a rigid substrate. When combined with a soft substrate, the Si material buckled from producing a wavy structure. The benefits of this Si-PDMS anode system are two-fold: the use of a compliant substrate solves the long-standing problem of the crippling stresses caused by large volumetric expansion and the out-of-plane buckling instability provides a means of accommodating large deformation during cyclic battery operation. The fundamental mechanism is that the structure released the stress by adjusting its buckling morphology, in effect avoiding fracture. The specific accomplishments of the work presented in this thesis are highlighted in this section.
The first analysis performed on a simple model consisting of beam elements to represent the Si film serves as a proof of concept for the stress relaxation hypothesis for this new Si anode in Li-ion batteries. Then a more rigorous study using only planar elements was performed in order to investigate the effect that Li insertion into a bulk Si material had on the morphology and evolution of stress. It was found that at a critical diffusion-induced strain the Si structure became unstable and buckled under developing compressive stresses. This however did not occur until a great deal of strain (lithiation) was experienced. The large expansion was accommodated by using the compliant substrate, and an order of magnitude of stress relaxation was seen at very high lithiation strains. The post-buckled morphology demonstrated a trend of constant wavelength and an amplitude that suddenly jumped after buckling initiated followed by a rather linear trend with the application of more diffusion-induced strain. A three-dimensional model was created in order to reduce the number of modeling assumptions, and this analysis too showed that buckling initiated after a critical threshold of strain, whereby the evolution of stress followed the familiar pattern seen in all previous analyses. Thus the hypothesis of using buckling as a means of stress relaxation is bolstered by the numerical work, and trends regarding the expected morphology of a one-dimensional wave can be discerned from this study.

As part of the aforementioned linear elastic analyses, a foray into the study of the effects of charge rate was performed. By applying a gradient of strain through the thickness of the Si material, it was found that uniform diffusion
through the Si material would provide the best performance in terms of stress relaxation. This is due to the fact that when the bottom portions of the Si material experience less deformation than the top region, the bottom layers serve as substrates in their own right, somewhat negating the benefits of the soft PDMS. Despite this, however, the short-diffusion lengths of Si thin films and nanostructures make this uniform diffusion very plausible for the duration of the entire battery operation. The analysis conducted indicated that thinner films are best, however logic suggests that there is an optimal dimension for the film thickness that will enable homogeneous diffusion while still benefiting from the stress relaxation due to buckling.

Due to recent experimental studies of the Si behavior under lithiation and de-lithiation which indicated plastic flow occurred during the charge and discharge cycles, further analysis of the Si-PDMS anode system was performed using a plastic material model in the planar model. The actual conditions and parameters of this plastic behavior are unknown, so the liberty was taken to study the behavior of an elastoplastic Si material qualitatively. Buckling was initiated as before; however the change in modulus due to the transition from elastic to plastic necessitated a change in the buckled morphology. The wavelength was subsequently reduced and the amplitude still increased with the applied lithiation strain but at a slower rate. The individual waves experienced increases in the local stress due to the change in morphology, but were subsequently unloaded as neighboring waves underwent to transition to plastic. Eventually the stress began to increase again, whereby the change in modulus of the Si film dictated a much
lower stress than the previous linear elastic cases and the elastoplastic analysis that incorporated a rigid substrate. Thus it is observed that the buckling of Si on a compliant substrate is still fundamentally dependent upon the ratio of the material properties and the design of the system with regard to boundary conditions.

Finally experimental evidence was produced in order to confirm the stress relaxation hypothesis. A preliminary test cell that incorporated Si ribbon anodes bonded to a PDMS substrate was electrochemically characterized, and its performance as well as the resulting morphology was assessed. After only a few cycles, the flat Si ribbons buckled into unique morphologies. The cyclic stability of the Si anodes on the elastomeric substrate is shown to fade to 3,500 mAh/g at 500 cycles, only 15% loss from the initial discharge cycle. This is a tremendous improvement above Li-ion batteries with Si anodes that have come before. This superior performance is attributed the fact that the Si ribbons buckled, which allowed them to relax the stress caused by the cyclic expansion and contraction due to lithiation and delithiation respectively.

6.2 Conclusions & Recommendations for Future Work

Stress relaxation via buckling of Si bonded to soft substrates for use as anodes has a great deal of promise for use in Li-ion batteries. Numerical studies have demonstrated that buckling will reduce the stress and that the plastic nature of the Si under lithiation will alter the buckled morphology. Experiments have confirmed the stress relaxation conjecture and have shown excellent cyclic stability and high performance. The experimental buckled geometry produces some unique variations, thus the morphology after cyclic charging/discharging
requires further study to determine what factors contribute to the evolution of the unique morphology. *In situ* observation and characterization of the Si ribbons is an immediate task that will help determine the factors that influence the resulting morphology and material behavior. From these observations perhaps some light can be shed upon the nonuniform Li concentration that has occurred during experimental studies of the Si anodes. The plastic nature of Si under the cyclic lithiation and delithiation has only been recently discovered and further investigation into this behavior is required for future numerical and experimental analysis. Additionally, work to understand the coupling between lithiation and deformation will help to bolster the thermal strain analogy and provide a more robust modeling method. The stress relaxation has been evidenced in both numerical and experimental analyses. This work serves as the first steps in solving one of the remaining bottlenecks in designing Si-based-anodes for high-performance Li-ion batteries to realize Si at its full potential. The results of this research encourage further work to systematically establish the optimal design criteria for the Si anodes such as the battery stability under a variety of conditions and the design envelope of the individual components of the cell for optimal performance. The researched contained in this thesis holds both fundamental and practical applications in the science community and battery industries.
REFERENCES


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Yu, Cunjiang, Xin Li, Jiepeng Rong, Teng Ma, Rongjun Zhang, Joseph Shaffer, Yonghao An, Qiang Liu, Bingqing Wei, and Hanqing Jiang. “Silicon Anodes on Soft Substrates in Lithium Ion Batteries: Stress Relaxation and High Performance.” *In Preparation*. (2011).


APPENDIX A

PATCH TEST RESULTS
For the planar study of the Si-PDMS anode system it is desired to use a combination of plane stress and plane strain elements, however it is not immediately clear how compatible these two elements are when used within the same analysis. A very common way to test the performance of elements under a variety of conditions is to conduct a patch test (Lepi, 1998). A patch test is designed to assess the results of a small "patch" of elements (Figure A.1) under sufficiently simple conditions and compare them to known values. A well designed patch test uses irregular elements of arbitrary geometry to avoid "lucky" results caused by symmetry, and at least one interior node (Irons, 1980 and MacNeal, 1994). There are two general types of patch tests that involve either specifying displacements on the exterior nodes to create a desired state of strain or specifying external loads to evaluate a desired state of stress (MacNeal, 1994). Another test exists to ensure that a rigid body motion (the same displacement applied to all exterior nodes) creates a stress-free and strain-free state by proving that the interior nodes displace by the same amount (NAFEMS, 1992). A patch test is either successful (at say six decimals) or it fails (Irons, 1980). Abaqus has a host of benchmark patch tests for all of its elements; however each patch test is designed for one type of element only. These tests have been performed and it has been verified that the plane stress and plane strain elements of interest, CPS4R and CPE4R respectively, pass their own patch tests.

A patch of 16 elements has been created in Abaqus (Figure A.2) that combines plane stress and plane strain elements. Because of the very different assumptions between plane stress and plane strain scenarios, the intent of this test
is to investigate a very simple model that incorporates both types of elements to
determine their compatibility. This will be done by employing a rigid body, a
displacement, and a thermal strain patch test. The top "layer" of elements is of
the plane stress formulation and the bottom is made up of plane strain elements.
Quadrilateral elements are used because they will be employed exclusively at the
interface of the Si and the PDMS. There are a total of four interior elements for
this patch test; two per each different element type. A first set of tests are
performed using the same material properties to determine the compatibility
between the two element types while a second set of tests uses material properties
similar to the proposed Si-PDMS anode system in order to study the effects these
differing properties will have on this simple simulation. The inside elements and
nodes in particular will be studied according to the procedure for a patch test
(MacNeal, 1994) to ensure the correct behavior of the entire model. The inside
elements are 4 and 5 for the top layer and 14 and 15 for the bottom layer. The
inside nodes are 101, 102, 103, 111, 112, and 113 for the plane strain elements
and 201, 202, 203, 211, 212, and 213 for the plane stress elements. Note that it is
an Abaqus convention to not report out-of-plane variables (stress, strain, etc.) for
plane stress elements (Abaqus Analysis User's Manual), therefore these components cannot be used for verification of the following patch tests.

![Diagram](image)

Figure A.2 Designed patch test of plane stress elements (top, red) and plane strain elements (bottom, blue) with (a) nodal labels and (b) element labels.

The first test is to verify that rigid body motion induces no strains or stresses within the patch. This means that if the exterior nodes are displaced by the same amount in the same direction, the displacement of the interior nodes will match their displacements exactly. A displacement boundary condition of $0.12 \cdot 10^{-3}$ is applied in both the horizontal and vertical directions to the exterior nodes only and it is verified that the patch remains stress and strain free (well within round-off tolerance) and that the interior nodes displace by $0.12 \cdot 10^{-3}$ in both directions as well.

The second test applies displacements to all exterior nodes of the form:

$$u = 10^{-3} \left( x + \frac{y}{2} \right)$$  \hspace{1cm} \text{(A.7)}$$

$$v = 10^{-3} \left( \frac{x}{2} + y \right)$$  \hspace{1cm} \text{(A.8)}$$
where \( u \) and \( v \) are the horizontal and vertical displacements respectively and \( x \) and \( y \) are the coordinates of the nodes. Note that node 10 will be fixed in its translational degrees of freedom because its coordinates are \( x=0 \) and \( y=0 \). The constraint of these two degrees of freedom is sufficient for this model because the planar elements have two translational degrees of freedom and no rotational degrees of freedom. The applied displacement field will create a field of constant strain (normal and shear strain) through the entire model of magnitude \( 10^{-3} \) according to the definition of strain as

\[
\varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \tag{A.9}
\]

The results from the displacement test show that indeed a state of constant strain is applied to the model and the deformation of the interior nodes corresponds to equation (A.7) and equation (A.8) exactly (Table A.1). The stress is computed according to Hooke's Law of isotropic materials for both plane stress,

\[
\sigma_{ij} = \frac{E}{1-\nu^2} \left[ (1-\nu)\varepsilon_{ij} + \nu \varepsilon_{kk} \delta_{ij} \right] \tag{A.10}
\]

and for plane strain,

\[
\sigma_{ij} = \frac{E}{(1+\nu)(1-2\nu)} \left[ (1-2\nu)\varepsilon_{ij} + \nu \varepsilon_{kk} \delta_{ij} \right] \tag{A.11}
\]

(Boresi, 2000) using the known, constant strain. The finite element results correspond with the analytical calculations exactly (Table A.2).

It is prudent to perform a test that will replicate the desired loading conditions a user wishes to employ to his/her actual model (MacNeal, 1994). A third test is designed to replicate the desired loading conditions for the Si-PDMS
Table A.1

Displacement Patch Test: Interior Nodal Displacements

<table>
<thead>
<tr>
<th>Node</th>
<th>FEA X-Disp. [10^{-3}]</th>
<th>Analytical X-Disp. [10^{-3}]</th>
<th>Error [%]</th>
<th>FEA Y-Disp. [10^{-3}]</th>
<th>Analytical Y-Disp. [10^{-3}]</th>
<th>Error [%]</th>
</tr>
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<td>0.115</td>
<td>0.00</td>
<td>0.095</td>
<td>0.095</td>
<td>0.00</td>
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<tr>
<td>102</td>
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<td>0.165</td>
<td>0.165</td>
<td>0.00</td>
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<tr>
<td>103</td>
<td>0.355</td>
<td>0.355</td>
<td>0.00</td>
<td>0.215</td>
<td>0.215</td>
<td>0.00</td>
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<td>0.140</td>
<td>0.00</td>
<td>0.145</td>
<td>0.145</td>
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<td>0.205</td>
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<td>0.290</td>
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<td>0.360</td>
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Table A.2

Displacement Patch Test: Element Stress

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<th>Element (Plane Strain)</th>
<th>Element 1-8</th>
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<td></td>
<td>FEA</td>
</tr>
<tr>
<td>( \sigma_{xx} )</td>
<td>1923</td>
</tr>
<tr>
<td>Error [%]</td>
<td>0.00</td>
</tr>
<tr>
<td>( \sigma_{yy} )</td>
<td>1923</td>
</tr>
<tr>
<td>Error [%]</td>
<td>0.00</td>
</tr>
<tr>
<td>( \tau_{xy} )</td>
<td>384.6</td>
</tr>
<tr>
<td>Error [%]</td>
<td>0.00</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Element (Plane Stress)</th>
<th>Element 11-18</th>
</tr>
</thead>
<tbody>
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<td>FEA</td>
</tr>
<tr>
<td>( \sigma_{xx} )</td>
<td>1429</td>
</tr>
<tr>
<td>Error [%]</td>
<td>0.00</td>
</tr>
<tr>
<td>( \sigma_{yy} )</td>
<td>1429</td>
</tr>
<tr>
<td>Error [%]</td>
<td>0.00</td>
</tr>
<tr>
<td>( \tau_{xy} )</td>
<td>384.6</td>
</tr>
<tr>
<td>Error [%]</td>
<td>0.00</td>
</tr>
</tbody>
</table>
simulations; a thermal strain. This test is broken into two parts; (a) the first applies a prescribed thermal strain (0.1%) to the top layer of plane stress elements only (Figure A.3a) and (b) the second applies an equivalent strain field by displacing all of the nodes in their base state by the amount that they are displaced from the first part. The motivation part (3a) of this test is to determine the suitability of using both element types in a simple simulation that utilizes a thermal strain as the loading. Since the displacement patch test succeeded without error, the second part, (3b), of this test serves as a benchmark to verify that the results from the first part satisfy the elastic theory (Figure A.3b). Nodes 10 and 30 are constrained in their motion in order to sufficiently prevent rigid body motions from occurring.

![Figure A.3 Schematic of the third patch test detailing the (a) thermal load applied to the top (plane stress elements) to produce stress and nodal deformations (dashed lines) and (b) the corresponding deformations (solid lines) applied to the same model to create an identical strain field.](image)

The displacements and the strains (Table A.3) from the thermal expansion test are recorded. The displacements are then placed upon all of the nodes for the second, verification analysis and the total strains at each element between both
parts are verified to be consistent with each other. The stress results from both parts of this third test are compared (Table A.4). The stress calculated in the presence of a thermal strains is

\[
\sigma_{ij} = \frac{E}{1-\nu^2} \left[ (1-\nu)\varepsilon_{ij} + \nu \varepsilon_{kk} \delta_{ij} - (1+\nu)\varepsilon_{TH} \right]
\]  \hspace{1cm} (A.12)

for plane stress, and

\[
\sigma_{ij} = \frac{E}{(1+\nu)(1-2\nu)} \left[ (1-2\nu)\varepsilon_{ij} + \nu \varepsilon_{kk} \delta_{ij} - (1+\nu)\varepsilon_{TH} \right]
\]  \hspace{1cm} (A.13)

for plane strain (Boresi, 2000), where \( \varepsilon_{TH} \) is the thermal strain calculated as the product of the coefficient of thermal expansion and the temperature. Since the total strain is the linear combination of the elastic and thermal strain (additive strain decomposition), the results from part (3a) less the stress caused by the thermal load (the last term of equations (A.12) and (A.13)) should match to the results of test (3b) exactly. The stress results from test (3a) match up with hand calculations exactly (see Appendix B). At 0.1% thermal strain using the modulus specified as \( 1 \times 10^6 \), the stress due to the thermal strain is -1430. Subtracting this value from the stresses of part (3a) give exactly those extracted from part (3b). Note that the stresses detailed for part (3b) are consistent with equations (A.10) and (A.11) for the strains reported by Abaqus.

The three aforementioned tests are repeated using two materials whose moduli are five orders of magnitude different (the same ratio as the moduli of Si to PDMS) in order to determine if any errors are introduced by using such different materials. All three tests for these differing materials passed with zero percent error just as reported however the results are not presented in detail here.
A full account of the calculations for all three tests along with the Abaqus input files can be found at the end of this appendix.

Table A.3

Total and Thermal Strain in Elements Due to Applied Thermal Strain as Reported by Abaqus for Test (3a)

<table>
<thead>
<tr>
<th>Element (Plane Strain)</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon_{xx}$ [10^{-4}]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>-1.04</td>
<td>-1.34</td>
<td>1.01</td>
<td>1.13</td>
<td>1.63</td>
<td>0.91</td>
<td>3.46</td>
<td>4.37</td>
</tr>
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<td>0.00</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
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<td>$\varepsilon_{yy}$ [10^{-4}]</td>
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<td></td>
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<td></td>
</tr>
<tr>
<td>Total</td>
<td>0.81</td>
<td>-0.11</td>
<td>-0.67</td>
<td>-0.11</td>
<td>-0.82</td>
<td>-0.24</td>
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<td></td>
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<td></td>
</tr>
<tr>
<td>$\varepsilon_{xy}$ [10^{-4}]</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>-0.23</td>
<td>1.31</td>
<td>-1.06</td>
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<td>-0.51</td>
<td>-2.65</td>
<td>-1.10</td>
<td>2.12</td>
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<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Element (Plane Stress)</th>
<th>11</th>
<th>12</th>
<th>13</th>
<th>14</th>
<th>15</th>
<th>16</th>
<th>17</th>
<th>18</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon_{xx}$ [10^{-4}]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td>6.68</td>
<td>6.11</td>
<td>8.72</td>
<td>9.39</td>
<td>8.51</td>
<td>8.75</td>
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<td>10.0</td>
<td>10.0</td>
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<td>10.0</td>
<td>10.0</td>
<td>10.0</td>
</tr>
<tr>
<td>$\varepsilon_{yy}$ [10^{-4}]</td>
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<td></td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
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<td>10.8</td>
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<td>$\varepsilon_{xy}$ [10^{-4}]</td>
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<tr>
<td>Total</td>
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<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
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</table>

The described patch tests have shown that using a combination of plane stress and plane strain elements will satisfactorily produce accurate results for the desired simulations. Further analyses are now carried out understanding that the different formulations of plane stress and plane strain elements will not bias the results. It should be noted for completeness that a simple test was performed involving the application of pressures on the exterior elements. This test to apply a stress to the model instead of an applied strain resulted in errors of less than 1% in general, however two elements had errors up to 9% with regard to the stress or the strain calculations. This type of patch test is not applicable for the simulation.
of diffusion induced strain in the Si-PDMS anode system, however, thus
subsequent analyses are carried in confidence due to the success of the three patch
tests discussed in the main text.

Table A.4

Stress Components In Elements Due to Applied Thermal Strain as Reported by
Abaqus for Tests (3a) and (3b)

<table>
<thead>
<tr>
<th>Element (Plane Strain)</th>
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<th>2</th>
<th>3</th>
<th>4</th>
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<th>7</th>
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<td>-187</td>
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<td>172</td>
<td>109</td>
<td>369</td>
<td>507</td>
</tr>
<tr>
<td>Part (3b)</td>
<td>-92.6</td>
<td>-187</td>
<td>97.1</td>
<td>146</td>
<td>172</td>
<td>109</td>
<td>369</td>
<td>507</td>
</tr>
<tr>
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<td>Part (3a)</td>
<td>-8.84</td>
<td>50.2</td>
<td>-40.8</td>
<td>92.1</td>
<td>-19.5</td>
<td>-102</td>
<td>-42.4</td>
<td>81.7</td>
</tr>
<tr>
<td>Part (3b)</td>
<td>-8.84</td>
<td>50.2</td>
<td>-40.8</td>
<td>92.1</td>
<td>-19.5</td>
<td>-102</td>
<td>-42.4</td>
<td>81.7</td>
</tr>
<tr>
<td>Error [%]</td>
<td>0.00</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Element (Plane Stress)</th>
<th>11</th>
<th>12</th>
<th>13</th>
<th>14</th>
<th>15</th>
<th>16</th>
<th>17</th>
<th>18</th>
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</thead>
<tbody>
<tr>
<td>σxx</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Part (3a)</td>
<td>-325</td>
<td>-404</td>
<td>-115</td>
<td>-74.1</td>
<td>-142</td>
<td>-136</td>
<td>118</td>
<td>196</td>
</tr>
<tr>
<td>Part (3a) Less Thermal Stress</td>
<td>1105</td>
<td>1026</td>
<td>1315</td>
<td>1356</td>
<td>1288</td>
<td>1294</td>
<td>1548</td>
<td>1626</td>
</tr>
<tr>
<td>Part (3b)</td>
<td>1105</td>
<td>1026</td>
<td>1315</td>
<td>1356</td>
<td>1288</td>
<td>1294</td>
<td>1548</td>
<td>1626</td>
</tr>
<tr>
<td>Error [%]</td>
<td>0.00</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>σyy</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Part (3a)</td>
<td>26.7</td>
<td>-48.3</td>
<td>45.1</td>
<td>-39.6</td>
<td>26.0</td>
<td>-31.8</td>
<td>-51.1</td>
<td>83.7</td>
</tr>
<tr>
<td>Part (3a) Less Thermal Stress</td>
<td>1457</td>
<td>1382</td>
<td>1475</td>
<td>1390</td>
<td>1456</td>
<td>1398</td>
<td>1379</td>
<td>1514</td>
</tr>
<tr>
<td>Part (3b)</td>
<td>1457</td>
<td>1382</td>
<td>1475</td>
<td>1390</td>
<td>1456</td>
<td>1398</td>
<td>1379</td>
<td>1514</td>
</tr>
<tr>
<td>Error [%]</td>
<td>0.00</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>σxy</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Part (3a)</td>
<td>-28.3</td>
<td>51.5</td>
<td>-49.0</td>
<td>48.0</td>
<td>-3.85</td>
<td>-95.7</td>
<td>-27.6</td>
<td>53.8</td>
</tr>
<tr>
<td>Part (3b)</td>
<td>-28.3</td>
<td>51.5</td>
<td>-49.0</td>
<td>48.0</td>
<td>-3.85</td>
<td>-95.7</td>
<td>-27.6</td>
<td>53.8</td>
</tr>
<tr>
<td>Error [%]</td>
<td>0.00</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
APPENDIX B

PATCH TEST INPUT AND CALCULATION FILES
B.1 Abaqus Input File

Contained in this section is the input file used to generate and perform the patch tests.

B.1.1 Patch Tests Using Same Material Properties

*HEADING
PLANE ELEM [CPS4R & CPE4R] PATCH TESTS (SAME MAT’L PROPS)
*PREPRINT,ECHO=YES,HISTORY=NO,MODEL=NO
**
**------ NODE CREATION ------**
*NODE
  10,0.00,0.00
  20,0.24,0.00
  30,0.36,0.00
  40,0.00,0.15
  50,0.20,0.15
  60,0.36,0.15
  70,0.00,0.30
  80,0.24,0.30
  90,0.36,0.30
  101,0.09,0.05
  102,0.21,0.06
  103,0.33,0.05
  111,0.09,0.10
  112,0.19,0.11
  113,0.31,0.11
  201,0.04,0.21
  202,0.18,0.20
  203,0.32,0.20
  211,0.06,0.26
  212,0.20,0.26
  213,0.32,0.24
**
**------ ELEMENT SPECIFICATION ------**
*ELEMENT,TYPE=CPE4R, ELSET=EPE
  1,10,20,102,101
  2,20,30,103,102
  3,10,101,111,40
  4,101,102,112,111
  5,102,103,113,112
  6,103,30,60,113
  7,111,112,50,40
  8,112,113,60,50
*ELEMENT,TYPE=CPS4R, ELSET=EPS
  11,40,50,202,201
  12,50,60,203,202
  13,40,201,211,70
  14,201,202,212,211
  15,202,203,213,212
**----- NODE SETS -----**
*NSET,NSET=SIDES,GENERATE
10,90,10
*NSET,NSET=TOP_NODE,GENERATE
40,90,10
201,203,1
211,213,1
**
**----- ELEMENT SETS -----**
*ELSET,ELSET=EALL,GENERATE
1,8,1
11,18,1
*ELSET,ELSET=EBOT,GENERATE
1,8,1
*ELSET,ELSET=ETOP,GENERATE
11,18,1
*ELSET,ELSET=CENTER_ELEM
4,5,14,15
**
**----- SECTIONS & MATERIALS -----**
*SOLID SECTION,MATERIAL=MAT1, ELSET=EBOT
.001,
*MATERIAL,NAME=MAT1
*ELASTIC,TYPE=ISOTROPIC
1.00E6,0.3
*EXPANSION
0.00
*SOLID SECTION,MATERIAL=MAT2, ELSET=ETOP
.001,
*MATERIAL,NAME=MAT2
*ELASTIC,TYPE=ISOTROPIC
1.00E6,0.3
*EXPANSION
2.6e-6
**
**------------------------**
**----- STEP 1: RIGID BODY -----**
**------------------------**
*STEP,PERTURBATION
*STATIC
*BOUNDARY
10,1,,0.12E-3
10,2,,0.12E-3
20,1,,0.12E-3
20,2,,0.12E-3
30,1,,0.12E-3
30,2,,0.12E-3
40,1,,0.12E-3
40,2,,0.12E-3
50,1,,0.12E-3
50,2,,0.12E-3
**-----------------------------------**
**----- STEP 2: CONSTANT STRAIN -----**
**-----------------------------------**

*ENERGY OUTPUT, VARIABLE=PRESELECT
*ENERGY PRINT
*EL PRINT
S,E
*EL PRINT, POSITION=NODES
S,E
*EL PRINT, POSITION=AVERAGED AT NODES
S,E
*EL PRINT, POSITION=CENTROID
S,E
*EL FILE
S,E

*OUTPUT, FIELD
*ELEMENT OUTPUT
S,E
*EL FILE, POSITION=NODES
S,E
*EL FILE, POSITION=AVERAGED AT NODES
S,E
*EL FILE, POSITION=CENTROID
S,E
*NODE PRINT, SUMMARY=NO
U,RF
*NODE FILE
U,RF
*END STEP
**
**-----------------------------------**

**------ STEP 2: CONSTANT STRAIN ------**
**-----------------------------------**

*STEP, PERTURBATION
*STATIC
*BOUNDARY
10,1,,0
10,2,,0
20,1,,0.240E-3
20,2,,0.120E-3
30,1,,0.360E-3
30,2,,0.180E-3
40,1,,0.075E-3
40,2,,0.150E-3
50,1,,0.275E-3
50,2,,0.250E-3
60,1,,0.435E-3
60,2,,0.330E-3
70,1,,0.150E-3
70,2,,0.300E-3
80,1,,0.390E-3
80,2,,0.420E-3
90,1,,0.510E-3
90,2,,0.480E-3
*ENERGY FILE
*OUTPUT,HISTORY,FREQUENCY=1
*ENERGY OUTPUT,VARIABLE=PRESSELECT
*ENERGY PRINT
*EL PRINT
S,E
*EL PRINT,POSITION=NODES
S,E
*EL PRINT,POSITION=AVERAGED AT NODES
S,E
*EL PRINT,POSITION=CENTROID
S,E
*EL FILE
S,E
*OUTPUT,FIELD
*ELEMENT OUTPUT
S,E
*EL FILE,POSITION=NODES
S,E
*EL FILE,POSITION=AVERAGED AT NODES
S,E
*EL FILE,POSITION=CENTROID
S,E
*NODE PRINT,SUMMARY=NO
U,RF
*NODE FILE
U,RF
*END STEP
**
**----------------------------------**
**----- STEP 3a: THERMAL STRAIN -----**
**----------------------------------**
*STEP
*STATIC
*TEMPERATURE
TOP_NODE,385
*BOUNDARY
10,1,2
30,2
*ENERGY PRINT
*ENERGY FILE
*OUTPUT,HISTORY,FREQUENCY=1
*ENERGY OUTPUT,VARIABLE=PRESSELECT
*EL PRINT,SUMMARY=NO
S,E
THE
*EL FILE
S,E
THE
*OUTPUT, FIELD
*ELEMENT OUTPUT
S,E
THE
*NODE PRINT, SUMMARY=NO
U,RF
*NODE FILE
U,RF
*OUTPUT, FIELD
U,RF
*NODE OUTPUT
U,RF
*END STEP
**
**------------------------------------------------**
**----- STEP 3b: EQUIVALENT STRAIN CHECK -----**
**----- APPLY DISPLACEMENTS FROM STEP 3a -----**
**------------------------------------------------**
*STEP, PERTURBATION
*STATIC
*BOUNDARY
10,1,, 0.000
10,2,, 0.000
20,1,, -6.5836E-05
20,2,, 8.8199E-05
30,1,, -1.0233E-04
30,2,, 0.000
40,1,, -1.4474E-04
40,2,, -1.6414E-05
50,1,, -4.5752E-05
50,2,, 7.9984E-05
60,1,, 3.6923E-05
60,2,, 7.1242E-06
70,1,, -2.8558E-04
70,2,, 1.4952E-04
80,1,, 1.3714E-05
80,2,, 2.3436E-04
90,1,, 1.6629E-04
90,2,, 1.5356E-04
101,1,, 6.8595E-05
101,2,, 4.1224E-05
102,1,, -4.3542E-05
102,2,, 7.6307E-05
103,1,, -4.5754E-05
103,2,, 4.1459E-05
111,1,, 5.8120E-05
111,2,, 4.4215E-05
112,1,, -5.8567E-05
112,2,, 6.6916E-05
113,1,, -1.8957E-05
113,2,, 5.0548E-05
201,1,, 1.8324E-04
201,2,, 7.7063E-05
202,1,, 5.0243E-05
202,2,, 1.1909E-04
203,1,, 5.0493E-05
203.2, 9.4840E-05
211.1, -1.7462E-04
211.2, 1.3966E-04
212.1, -4.2999E-05
212.2, 1.7750E-04
213.1, 7.4674E-05
213.2, 1.4031E-04
*ENERGY FILE
*OUTPUT,HISTORY,FREQUENCY=1
*ENERGY OUTPUT,VARIABLE=PRESELECT
*ENERGY PRINT
*EL PRINT
  S,E
*EL PRINT,POSITION=NODES
  S,E
*EL PRINT,POSITION=AVERAGED AT NODES
  S,E
*EL PRINT,POSITION=CENTROID
  S,E
*EL FILE
  S,E
*OUTPUT,FIELD
*ELEMENT OUTPUT
  S,E
*EL FILE,POSITION=NODES
  S,E
*EL FILE,POSITION=AVERAGED AT NODES
  S,E
*EL FILE,POSITION=CENTROID
  S,E
*NODE PRINT,SUMMARY=NO
  U,RF
*NODE FILE
  U,RF
*END STEP
B.1.2 Patch Tests Using Different Material Properties

The input file for the patch test of different material properties is identical to the previous input script, however the input lines for the property definition have changed as such:

```plaintext
*--- SECTIONS & MATERIALS ---*
*SOLID SECTION,MATERIAL=MAT1, ELSET=EBOT
 .001,
*MATERIAL,NAME=MAT1
*ELASTIC,TYPE=ISOTROPIC
 15,0.495
*EXPANSION
 0.00
*SOLID SECTION,MATERIAL=MAT2, ELSET=ETOP
 .001,
*MATERIAL,NAME=MAT2
*ELASTIC,TYPE=ISOTROPIC
 1.00E6,0.3
*EXPANSION
 2.6e-6
```

The remainder of the input file is not printed here for brevity.
B.2 MathCAD Calculation Sheets

Contained in this section are the calculation sheets used to verify the patch tests.

B.2.1 MathCAD Calculation sheets – Same Material Properties

Combined Plane-Stress/Plane-Strain Patch Test Calculations

Analysis Constants

Node Coordinates - Bottom Layer

\[
\begin{align*}
x_{10} &= 0.00 & y_{10} &= 0.00 & x_{101} &= 0.09 & y_{101} &= 0.05 & x_{111} &= 0.09 & y_{111} &= 0.10 \\
x_{20} &= 0.24 & y_{20} &= 0.00 & x_{102} &= 0.21 & y_{102} &= 0.06 & x_{112} &= 0.19 & y_{112} &= 0.11 \\
x_{30} &= 0.36 & y_{30} &= 0.00 & x_{103} &= 0.33 & y_{103} &= 0.05 & x_{113} &= 0.31 & y_{113} &= 0.11 \\
\end{align*}
\]

Node Coordinates - Interface

\[
\begin{align*}
x_{40} &= 0.00 & y_{40} &= 0.15 \\
x_{50} &= 0.20 & y_{50} &= 0.15 \\
x_{60} &= 0.36 & y_{60} &= 0.15 \\
\end{align*}
\]

Node Coordinates - Top Layer

\[
\begin{align*}
x_{70} &= 0.00 & y_{70} &= 0.30 & x_{201} &= 0.04 & y_{201} &= 0.21 & x_{211} &= 0.06 & y_{211} &= 0.26 \\
x_{80} &= 0.24 & y_{80} &= 0.30 & x_{202} &= 0.18 & y_{202} &= 0.20 & x_{212} &= 0.20 & y_{212} &= 0.26 \\
x_{90} &= 0.36 & y_{90} &= 0.30 & x_{203} &= 0.32 & y_{203} &= 0.20 & x_{213} &= 0.32 & y_{213} &= 0.24 \\
\end{align*}
\]

Material Properties

Bottom Layer (Plane Strain)

\[
E_1 := 1 \cdot 10^6 \quad \nu_1 := 0.3 \quad G_1 := \frac{E_1}{2(1 + \nu_1)} = 3.846 \times 10^5
\]

Top Layer (Plane Stress)

\[
E_2 := 1 \cdot 10^6 \quad \nu_2 := 0.3 \quad G_2 := \frac{E_2}{2(1 + \nu_2)} = 3.846 \times 10^5
\]

\[
\alpha_2 := 2.6 \cdot 10^{-6}
\]
Test #2: Displacement Patch Test

Exterior Node Deformations

\[
\begin{align*}
\text{u10} &= 10^{-3} \left( x_{10} + \frac{y_{10}}{2} \right) = 0 \\
\text{v10} &= 10^{-3} \left( y_{10} + \frac{x_{10}}{2} \right) = 0 \\
\text{u20} &= 10^{-3} \left( x_{20} + \frac{y_{20}}{2} \right) = 2.4 \times 10^{-4} \\
\text{v20} &= 10^{-3} \left( y_{20} + \frac{x_{20}}{2} \right) = 1.2 \times 10^{-4} \\
\text{u30} &= 10^{-3} \left( x_{30} + \frac{y_{30}}{2} \right) = 3.6 \times 10^{-4} \\
\text{v30} &= 10^{-3} \left( y_{30} + \frac{x_{30}}{2} \right) = 1.8 \times 10^{-4} \\
\text{u40} &= 10^{-3} \left( x_{40} + \frac{y_{40}}{2} \right) = 7.5 \times 10^{-5} \\
\text{v40} &= 10^{-3} \left( y_{40} + \frac{x_{40}}{2} \right) = 1.5 \times 10^{-4} \\
\text{u50} &= 10^{-3} \left( x_{50} + \frac{y_{50}}{2} \right) = 2.75 \times 10^{-4} \\
\text{v50} &= 10^{-3} \left( y_{50} + \frac{x_{50}}{2} \right) = 2.5 \times 10^{-4} \\
\text{u60} &= 10^{-3} \left( x_{60} + \frac{y_{60}}{2} \right) = 4.35 \times 10^{-4} \\
\text{v60} &= 10^{-3} \left( y_{60} + \frac{x_{60}}{2} \right) = 3.3 \times 10^{-4} \\
\text{u70} &= 10^{-3} \left( x_{70} + \frac{y_{70}}{2} \right) = 1.5 \times 10^{-4} \\
\text{v70} &= 10^{-3} \left( y_{70} + \frac{x_{70}}{2} \right) = 3 \times 10^{-4} \\
\text{u80} &= 10^{-3} \left( x_{80} + \frac{y_{80}}{2} \right) = 3.9 \times 10^{-4} \\
\text{v80} &= 10^{-3} \left( y_{80} + \frac{x_{80}}{2} \right) = 4.2 \times 10^{-4} \\
\text{u90} &= 10^{-3} \left( x_{90} + \frac{y_{90}}{2} \right) = 5.1 \times 10^{-4} \\
\text{v90} &= 10^{-3} \left( y_{90} + \frac{x_{90}}{2} \right) = 4.8 \times 10^{-4}
\end{align*}
\]
Calculated Interior Node Deformations

\[
\begin{align*}
\mathbf{u}_{101} &= 10^{-3} \left( x_{101} + \frac{y_{101}}{2} \right) = 1.15 \times 10^{-4} \\
\mathbf{u}_{102} &= 10^{-3} \left( x_{102} + \frac{y_{102}}{2} \right) = 2.4 \times 10^{-4} \\
\mathbf{u}_{103} &= 10^{-3} \left( x_{103} + \frac{y_{103}}{2} \right) = 3.55 \times 10^{-4} \\
\mathbf{u}_{111} &= 10^{-3} \left( x_{111} + \frac{y_{111}}{2} \right) = 1.4 \times 10^{-4} \\
\mathbf{u}_{112} &= 10^{-3} \left( x_{112} + \frac{y_{112}}{2} \right) = 2.45 \times 10^{-4} \\
\mathbf{u}_{113} &= 10^{-3} \left( x_{113} + \frac{y_{113}}{2} \right) = 3.65 \times 10^{-4} \\
\mathbf{u}_{201} &= 10^{-3} \left( x_{201} + \frac{y_{201}}{2} \right) = 1.45 \times 10^{-4} \\
\mathbf{u}_{202} &= 10^{-3} \left( x_{202} + \frac{y_{202}}{2} \right) = 2.8 \times 10^{-4} \\
\mathbf{u}_{203} &= 10^{-3} \left( x_{203} + \frac{y_{203}}{2} \right) = 4.2 \times 10^{-4} \\
\mathbf{u}_{211} &= 10^{-3} \left( x_{211} + \frac{y_{211}}{2} \right) = 1.9 \times 10^{-4} \\
\mathbf{u}_{212} &= 10^{-3} \left( x_{212} + \frac{y_{212}}{2} \right) = 3.3 \times 10^{-4} \\
\mathbf{u}_{213} &= 10^{-3} \left( x_{213} + \frac{y_{213}}{2} \right) = 4.4 \times 10^{-4}
\end{align*}
\]

\[
\begin{align*}
\mathbf{v}_{101} &= 10^{-3} \left( y_{101} + \frac{x_{101}}{2} \right) = 9.5 \times 10^{-5} \\
\mathbf{v}_{102} &= 10^{-3} \left( y_{102} + \frac{x_{102}}{2} \right) = 1.65 \times 10^{-4} \\
\mathbf{v}_{103} &= 10^{-3} \left( y_{103} + \frac{x_{103}}{2} \right) = 2.15 \times 10^{-4} \\
\mathbf{v}_{111} &= 10^{-3} \left( y_{111} + \frac{x_{111}}{2} \right) = 1.45 \times 10^{-4} \\
\mathbf{v}_{112} &= 10^{-3} \left( y_{112} + \frac{x_{112}}{2} \right) = 2.05 \times 10^{-4} \\
\mathbf{v}_{113} &= 10^{-3} \left( y_{113} + \frac{x_{113}}{2} \right) = 2.65 \times 10^{-4} \\
\mathbf{v}_{201} &= 10^{-3} \left( y_{201} + \frac{x_{201}}{2} \right) = 2.3 \times 10^{-4} \\
\mathbf{v}_{202} &= 10^{-3} \left( y_{202} + \frac{x_{202}}{2} \right) = 2.9 \times 10^{-4} \\
\mathbf{v}_{203} &= 10^{-3} \left( y_{203} + \frac{x_{203}}{2} \right) = 3.6 \times 10^{-4} \\
\mathbf{v}_{211} &= 10^{-3} \left( y_{211} + \frac{x_{211}}{2} \right) = 2.9 \times 10^{-4} \\
\mathbf{v}_{212} &= 10^{-3} \left( y_{212} + \frac{x_{212}}{2} \right) = 3.6 \times 10^{-4} \\
\mathbf{v}_{213} &= 10^{-3} \left( y_{213} + \frac{x_{213}}{2} \right) = 4 \times 10^{-4}
\end{align*}
\]
Stress Calculations

Applied Strain

\[ \varepsilon_{xx} = 10^{-3} \quad \varepsilon_{yy} = 10^{-3} \quad \varepsilon_{xy} = 10^{-3} \]

\[ \mathbf{\varepsilon} = \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{xy} / 2 \end{pmatrix} = \begin{pmatrix} 1 \times 10^{-3} \\ 1 \times 10^{-3} \\ 5 \times 10^{-4} \end{pmatrix} \]

Calculated Stress - Bottom Layer (Plane Strain)

\[ \sigma = \frac{E_1}{(1 + v_1)(1 - 2v_1)} \begin{pmatrix} 1 - v_1 & v_1 & 0 \\ v_1 & 1 - v_1 & 0 \\ 0 & 0 & 1 - 2v_1 \end{pmatrix} \cdot \mathbf{\varepsilon} = \begin{pmatrix} 1923.08 \\ 1923.08 \\ 384.62 \end{pmatrix} \]

Calculated Stress - Top Layer (Plane Stress)

\[ \sigma = \frac{E_2}{(1 - v_2^2)} \begin{pmatrix} 1 & v_2 & 0 \\ v_2 & 1 & 0 \\ 0 & 0 & 1 - v_2 \end{pmatrix} \cdot \mathbf{\varepsilon} = \begin{pmatrix} 1429 \\ 1429 \\ 385 \end{pmatrix} \]
Test #3a: Thermal Strain Patch Test

Total Strain in Each Element As Reported by Abaqus

\[
\begin{align*}
\varepsilon_1 & := \begin{pmatrix} e_{xx1} \\
 e_{yy1} \\
 e_{xy1} \\
\end{pmatrix} = \begin{pmatrix} -1.036 \times 10^{-4} \\
 8.109 \times 10^{-5} \\
-1.149 \times 10^{-5} \\
\end{pmatrix}, & \varepsilon_{11} & := \begin{pmatrix} e_{xx11} \\
 e_{yy11} \\
 e_{xy11} \\
\end{pmatrix} = \begin{pmatrix} 6.677 \times 10^{-4} \\
 1.125 \times 10^{-3} \\
-3.682 \times 10^{-5} \\
\end{pmatrix}
\end{align*}
\]

\[
\begin{align*}
\varepsilon_2 & := \begin{pmatrix} e_{xx2} \\
 e_{yy2} \\
 e_{xy2} \\
\end{pmatrix} = \begin{pmatrix} -1.345 \times 10^{-4} \\
-1.111 \times 10^{-5} \\
 6.525 \times 10^{-5} \\
\end{pmatrix}, & \varepsilon_{12} & := \begin{pmatrix} e_{xx12} \\
 e_{yy12} \\
 e_{xy12} \\
\end{pmatrix} = \begin{pmatrix} 6.114 \times 10^{-4} \\
 1.074 \times 10^{-3} \\
 6.695 \times 10^{-5} \\
\end{pmatrix}
\end{align*}
\]

\[
\begin{align*}
\varepsilon_3 & := \begin{pmatrix} e_{xx3} \\
 e_{yy3} \\
 e_{xy3} \\
\end{pmatrix} = \begin{pmatrix} 1.009 \times 10^{-4} \\
-6.711 \times 10^{-5} \\
-5.308 \times 10^{-5} \\
\end{pmatrix}, & \varepsilon_{13} & := \begin{pmatrix} e_{xx13} \\
 e_{yy13} \\
 e_{xy13} \\
\end{pmatrix} = \begin{pmatrix} 8.723 \times 10^{-4} \\
 1.081 \times 10^{-3} \\
-6.37 \times 10^{-5} \\
\end{pmatrix}
\end{align*}
\]

\[
\begin{align*}
\varepsilon_4 & := \begin{pmatrix} e_{xx4} \\
 e_{yy4} \\
 e_{xy4} \\
\end{pmatrix} = \begin{pmatrix} 1.134 \times 10^{-4} \\
-1.126 \times 10^{-5} \\
 1.198 \times 10^{-4} \\
\end{pmatrix}, & \varepsilon_{14} & := \begin{pmatrix} e_{xx14} \\
 e_{yy14} \\
 e_{xy14} \\
\end{pmatrix} = \begin{pmatrix} 9.387 \times 10^{-4} \\
 9.836 \times 10^{-4} \\
 6.241 \times 10^{-5} \\
\end{pmatrix}
\end{align*}
\]

\[
\begin{align*}
\varepsilon_5 & := \begin{pmatrix} e_{xx5} \\
 e_{yy5} \\
 e_{xy5} \\
\end{pmatrix} = \begin{pmatrix} 1.627 \times 10^{-4} \\
-8.159 \times 10^{-5} \\
-2.53 \times 10^{-5} \\
\end{pmatrix}, & \varepsilon_{15} & := \begin{pmatrix} e_{xx15} \\
 e_{yy15} \\
 e_{xy15} \\
\end{pmatrix} = \begin{pmatrix} 8.511 \times 10^{-4} \\
 1.07 \times 10^{-3} \\
-5.004 \times 10^{-6} \\
\end{pmatrix}
\end{align*}
\]

\[
\begin{align*}
\varepsilon_6 & := \begin{pmatrix} e_{xx6} \\
 e_{yy6} \\
 e_{xy6} \\
\end{pmatrix} = \begin{pmatrix} 9.124 \times 10^{-5} \\
-2.413 \times 10^{-5} \\
-1.323 \times 10^{-4} \\
\end{pmatrix}, & \varepsilon_{16} & := \begin{pmatrix} e_{xx16} \\
 e_{yy16} \\
 e_{xy16} \\
\end{pmatrix} = \begin{pmatrix} 8.746 \times 10^{-4} \\
 1.01 \times 10^{-3} \\
-1.244 \times 10^{-4} \\
\end{pmatrix}
\end{align*}
\]

\[
\begin{align*}
\varepsilon_7 & := \begin{pmatrix} e_{xx7} \\
 e_{yy7} \\
 e_{xy7} \\
\end{pmatrix} = \begin{pmatrix} 3.456 \times 10^{-4} \\
-1.705 \times 10^{-4} \\
-5.511 \times 10^{-5} \\
\end{pmatrix}, & \varepsilon_{17} & := \begin{pmatrix} e_{xx17} \\
 e_{yy17} \\
 e_{xy17} \\
\end{pmatrix} = \begin{pmatrix} 1.134 \times 10^{-3} \\
 9.146 \times 10^{-4} \\
-3.587 \times 10^{-5} \\
\end{pmatrix}
\end{align*}
\]

\[
\begin{align*}
\varepsilon_8 & := \begin{pmatrix} e_{xx8} \\
 e_{yy8} \\
 e_{xy8} \\
\end{pmatrix} = \begin{pmatrix} 4.367 \times 10^{-4} \\
-1.404 \times 10^{-4} \\
 1.062 \times 10^{-4} \\
\end{pmatrix}, & \varepsilon_{18} & := \begin{pmatrix} e_{xx18} \\
 e_{yy18} \\
 e_{xy18} \\
\end{pmatrix} = \begin{pmatrix} 1.172 \times 10^{-3} \\
 1.026 \times 10^{-3} \\
 6.996 \times 10^{-5} \\
\end{pmatrix}
\end{align*}
\]
Stress Calculations

Calculated Stress - Bottom Layer (Plane Strain)

\[
\sigma_1 = \frac{E_1}{(1 + \nu_1)(1 - 2\nu_1)} \begin{pmatrix} 1 - \nu_1 & \nu_1 & 0 \\ \nu_1 & 1 - \nu_1 & 0 \\ 0 & 0 & 1 - 2\nu_1 \end{pmatrix} \cdot \varepsilon_1 = \begin{pmatrix} -92.6 \\ 49.4 \\ -8.8 \end{pmatrix}
\]

\[
\sigma_2 = \frac{E_1}{(1 + \nu_1)(1 - 2\nu_1)} \begin{pmatrix} 1 - \nu_1 & \nu_1 & 0 \\ \nu_1 & 1 - \nu_1 & 0 \\ 0 & 0 & 1 - 2\nu_1 \end{pmatrix} \cdot \varepsilon_2 = \begin{pmatrix} -187.4 \\ -92.5 \\ 50.2 \end{pmatrix}
\]

\[
\sigma_3 = \frac{E_1}{(1 + \nu_1)(1 - 2\nu_1)} \begin{pmatrix} 1 - \nu_1 & \nu_1 & 0 \\ \nu_1 & 1 - \nu_1 & 0 \\ 0 & 0 & 1 - 2\nu_1 \end{pmatrix} \cdot \varepsilon_3 = \begin{pmatrix} 97.1 \\ -32.1 \\ -40.8 \end{pmatrix}
\]

\[
\sigma_4 = \frac{E_1}{(1 + \nu_1)(1 - 2\nu_1)} \begin{pmatrix} 1 - \nu_1 & \nu_1 & 0 \\ \nu_1 & 1 - \nu_1 & 0 \\ 0 & 0 & 1 - 2\nu_1 \end{pmatrix} \cdot \varepsilon_4 = \begin{pmatrix} 146.2 \\ 50.3 \\ 92.1 \end{pmatrix}
\]

\[
\sigma_5 = \frac{E_1}{(1 + \nu_1)(1 - 2\nu_1)} \begin{pmatrix} 1 - \nu_1 & \nu_1 & 0 \\ \nu_1 & 1 - \nu_1 & 0 \\ 0 & 0 & 1 - 2\nu_1 \end{pmatrix} \cdot \varepsilon_5 = \begin{pmatrix} 172 \\ -15.9 \\ -19.5 \end{pmatrix}
\]

\[
\sigma_6 = \frac{E_1}{(1 + \nu_1)(1 - 2\nu_1)} \begin{pmatrix} 1 - \nu_1 & \nu_1 & 0 \\ \nu_1 & 1 - \nu_1 & 0 \\ 0 & 0 & 1 - 2\nu_1 \end{pmatrix} \cdot \varepsilon_6 = \begin{pmatrix} 108.9 \\ 20.1 \\ -101.8 \end{pmatrix}
\]

\[
\sigma_7 = \frac{E_1}{(1 + \nu_1)(1 - 2\nu_1)} \begin{pmatrix} 1 - \nu_1 & \nu_1 & 0 \\ \nu_1 & 1 - \nu_1 & 0 \\ 0 & 0 & 1 - 2\nu_1 \end{pmatrix} \cdot \varepsilon_7 = \begin{pmatrix} 366.8 \\ -30.2 \\ -42.4 \end{pmatrix}
\]

\[
\sigma_8 = \frac{E_1}{(1 + \nu_1)(1 - 2\nu_1)} \begin{pmatrix} 1 - \nu_1 & \nu_1 & 0 \\ \nu_1 & 1 - \nu_1 & 0 \\ 0 & 0 & 1 - 2\nu_1 \end{pmatrix} \cdot \varepsilon_8 = \begin{pmatrix} 506.9 \\ 62.9 \\ 81.7 \end{pmatrix}
\]
Calculated Stress - Top Layer (Plane Stress)

Applied Thermal Strain

\[ \varepsilon_{TH} := 385 \cdot \alpha 2 = 0.001 \]

\[
\begin{align*}
\sigma_{11} := & \frac{E_2}{(1 - \nu^2)} \begin{pmatrix} 1 & \nu^2 & 0 \\ \nu^2 & 1 & 0 \\ 0 & 0 & 1 - \nu^2 \end{pmatrix} \varepsilon_{11} - \frac{E_2}{(1 - \nu^2)}(1 + \nu^2) \begin{pmatrix} \varepsilon_{TH} \\ 0 \end{pmatrix} = \begin{pmatrix} -325.3 \\ 26.6 \\ -28.3 \end{pmatrix} \\
\sigma_{12} := & \frac{E_2}{(1 - \nu^2)} \begin{pmatrix} 1 & \nu^2 & 0 \\ \nu^2 & 1 & 0 \\ 0 & 0 & 1 - \nu^2 \end{pmatrix} \varepsilon_{12} - \frac{E_2}{(1 - \nu^2)}(1 + \nu^2) \begin{pmatrix} \varepsilon_{TH} \\ 0 \end{pmatrix} = \begin{pmatrix} -404.1 \\ -48.2 \\ 51.5 \end{pmatrix} \\
\sigma_{13} := & \frac{E_2}{(1 - \nu^2)} \begin{pmatrix} 1 & \nu^2 & 0 \\ \nu^2 & 1 & 0 \\ 0 & 0 & 1 - \nu^2 \end{pmatrix} \varepsilon_{13} - \frac{E_2}{(1 - \nu^2)}(1 + \nu^2) \begin{pmatrix} \varepsilon_{TH} \\ 0 \end{pmatrix} = \begin{pmatrix} -115.2 \\ 45.2 \\ -49 \end{pmatrix} \\
\sigma_{14} := & \frac{E_2}{(1 - \nu^2)} \begin{pmatrix} 1 & \nu^2 & 0 \\ \nu^2 & 1 & 0 \\ 0 & 0 & 1 - \nu^2 \end{pmatrix} \varepsilon_{14} - \frac{E_2}{(1 - \nu^2)}(1 + \nu^2) \begin{pmatrix} \varepsilon_{TH} \\ 0 \end{pmatrix} = \begin{pmatrix} -74.1 \\ -39.6 \\ 48 \end{pmatrix} \\
\sigma_{15} := & \frac{E_2}{(1 - \nu^2)} \begin{pmatrix} 1 & \nu^2 & 0 \\ \nu^2 & 1 & 0 \\ 0 & 0 & 1 - \nu^2 \end{pmatrix} \varepsilon_{15} - \frac{E_2}{(1 - \nu^2)}(1 + \nu^2) \begin{pmatrix} \varepsilon_{TH} \\ 0 \end{pmatrix} = \begin{pmatrix} -142.1 \\ 26.1 \\ -3.8 \end{pmatrix} \\
\sigma_{16} := & \frac{E_2}{(1 - \nu^2)} \begin{pmatrix} 1 & \nu^2 & 0 \\ \nu^2 & 1 & 0 \\ 0 & 0 & 1 - \nu^2 \end{pmatrix} \varepsilon_{16} - \frac{E_2}{(1 - \nu^2)}(1 + \nu^2) \begin{pmatrix} \varepsilon_{TH} \\ 0 \end{pmatrix} = \begin{pmatrix} -136 \\ -31.8 \\ -95.7 \end{pmatrix} \\
\sigma_{17} := & \frac{E_2}{(1 - \nu^2)} \begin{pmatrix} 1 & \nu^2 & 0 \\ \nu^2 & 1 & 0 \\ 0 & 0 & 1 - \nu^2 \end{pmatrix} \varepsilon_{17} - \frac{E_2}{(1 - \nu^2)}(1 + \nu^2) \begin{pmatrix} \varepsilon_{TH} \\ 0 \end{pmatrix} = \begin{pmatrix} 117.7 \\ -51 \\ -27.6 \end{pmatrix} \\
\sigma_{18} := & \frac{E_2}{(1 - \nu^2)} \begin{pmatrix} 1 & \nu^2 & 0 \\ \nu^2 & 1 & 0 \\ 0 & 0 & 1 - \nu^2 \end{pmatrix} \varepsilon_{18} - \frac{E_2}{(1 - \nu^2)}(1 + \nu^2) \begin{pmatrix} \varepsilon_{TH} \\ 0 \end{pmatrix} = \begin{pmatrix} 195.7 \\ 83.7 \\ 53.8 \end{pmatrix}
\end{align*}
\]
B.2.2 MathCAD Calculation sheets – Different Material Properties

The MathCAD calculations for the patch test of different material properties are identical to the previous calculations, however the corresponding materials have changed and the results are checked against the Abaqus data. A 100% correlation is observed between the hand calculations and the FE results. These calculations and results comparisons are not presented here for brevity.
APPENDIX C

MESH CONVERGENCE TEST RESULTS
In order to achieve the best accuracy at an economical cost (i.e. computational time) a mesh convergence study is performed. This study uses local mesh refinement of the Si material and at the Si-PDMS interface because the stress within the Si material is of great concern for this study and the far-away elements serve only to represent geometry and transmit load ("The Importance of Mesh Convergence," 2010). The meshing strategy is as follows: the Si thin-film is partitioned into four layers, the Si thin-film is meshed along its length with five different divisions (1000, 2000, 3000, 4000, and 5000) and four elements through its thickness, the PDMS adjacent to the Si thin-film is meshed along the length with the same number of elements as the Si (to achieve coincident nodes) that have an aspect ratio of one, and then the PDMS is partitioned with elements of increasing size (but still aspect ratio of one) from the interface to the base as discussed previously (Figure C.1). Since the number of Si elements through its thickness remains constant, the aspect ratio, calculated as the ratio of an element's thickness to its length (i.e. \( \Delta y/\Delta x \)) will increase to unity with each refinement of the mesh (Table C.1). The ideal number of elements through the thickness should be a minimum of three in order to capture the compressive, tensile, and neutral zones that are prevalent for a state that is predominantly bending. The aforementioned challenge of meshing this system in the presence of the large difference in thicknesses becomes more of an issue now. Maintaining sufficiently small aspect ratios of the Si elements requires a finer mesh along the length, which requires a reduction in the size of the elements of the PDMS near the interfacial region. A study investigating more elements (more than four) through
the Si thickness at the same aspect ratios is computationally prohibitive because the mesh must be identical between the Si and PDMS. It is assumed that sufficiently accurate results for the stress can be obtained with four elements through the Si thickness. In order to accommodate the necessity of finer meshing of the Si down its length while preserving acceptable aspect ratios, the PDMS is partitioned further near the interface, almost two-fold compared to the mesh of the proof of concept, in order to help reduce the overall number of elements while retaining fidelity of the simulation results.

Figure C.1 The meshing strategy used for convergence testing where the Si material is meshed with CPS4R elements at varying levels of refinement down its length, the PDMS material is meshed with CPE4R elements with unit aspect ratio and CPE3 elements at the transition zones, a well-established method (NAFEMS, 1992), in order to gradually increase the element size away from the Si-PDMS interface.

The geometry of the Si film is 100 nm thin by 300 μm long and the PDMS is 750 μm thick by 300 μm long. The analysis methodology is the same as previously described, where the base of the PDMS is constrained in its translational degrees of freedom and the applied load is a thermal strain of the Si thin-film only. The criteria for determining convergence that will be used include
comparison of stress at several locations of the Si material and of the film morphology (wavelength and amplitude).

Table C.1
Mesh Convergence Study Element Statistics

<table>
<thead>
<tr>
<th>Case</th>
<th>Si Thin-Film Elements</th>
<th>PDMS Substrate</th>
<th>Net Total Elements</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Thickness</td>
<td>Length</td>
<td>Total No. of Elements</td>
</tr>
<tr>
<td>1</td>
<td>4</td>
<td>1,000</td>
<td>4,000</td>
</tr>
<tr>
<td>2</td>
<td>4</td>
<td>2,000</td>
<td>8,000</td>
</tr>
<tr>
<td>3</td>
<td>4</td>
<td>3,000</td>
<td>12,000</td>
</tr>
<tr>
<td>4</td>
<td>4</td>
<td>4,000</td>
<td>16,000</td>
</tr>
<tr>
<td>5</td>
<td>4</td>
<td>5,000</td>
<td>20,000</td>
</tr>
</tbody>
</table>

The results of this mesh convergence study are as expected; with a refined mesh, or the results converge to a solution with decreasing error. As can be seen by the plot of stress as a function strain, the difference between Case 3, Case 4, and Case 5 is indiscernible (Figure C.2a). This plot is typical of the stress evaluated at four different locations (peaks and valleys). Note that with improved aspect ratios (closer to unity) the percent error in the measured stress calculated according to

$$
\text{error}_{\%} = \left| \frac{\sigma_{VMi}^{n+1} - \sigma_{VMi}^{n}}{\sigma_{VMi}^{n+1}} \right| \cdot 100
$$

(C.14)

where $\sigma_{VM}$ is the von Mises equivalent stress evaluated at the $i^{th}$ strain for the $n^{th}$ increment in mesh refinement, decreases from approximately 10% from Case 1 to Case 2, less than 1% from Case 3 to Case 4, and less than 0.1% from Case 4 to Case 5 (Figure C.2b). Based upon the results for the stress in the Si material, an
appropriate mesh density within reasonable accuracy for this system is Case 3. The von Mises stress is used as a measure of failure of the Si material, however it is noted here that the von Mises stress is composed primarily by the normal stress in the x-direction (direction along Si film's length). This is the bending stress caused by buckling.

The average wavelength of six waves and the average amplitudes of eight waves are both measured at several strains and normalized by the Si thickness for the five cases of this convergence study. There is no appreciable change in these measurements from one case to the other (Figure C.3). The error bars of the plots correspond to ±2 standard deviations of the averaged measurements, and indicate that in general the most error occurs at lower strains when the structure first begins to buckle.

Figure C.2 Mesh convergence study for (a) stress at the outer fibers of the Si material with negligible difference between the last three cases and (b) analysis of stress at several strains as the mesh is refined.

Based upon this analysis, the mesh specified by Case 3 is the most appropriate for future analysis. It is determined that the stresses converge to within <1% at this mesh density. The measurements of deformation (i.e.
wavelength and amplitude) do not vary much even at the coarsest mesh, which is to be expected (NAFEMS, 1992). However the deviation is observed to be less for Cases 3 through 5 (especially for wavelength) due to the greater degree of discretization. Unless otherwise specified, the geometry and mesh density of Case 3 detailed in this section will be that of the analyses discussed in all sections of the main text.

Figure C.3 Mesh convergence study based upon buckled morphology showing accurate results are obtained and that little change in morphology occurs due to mesh refinement.
When solving nonlinear problems, Abaqus will increment the load step automatically. For highly nonlinear problems, the increment size is reduced until a solution is achieved. Failure to reach a solution within a threshold of increment size (as defined by the user) results in a failure to converge and the analysis stops. Some nonlinear problems are very unstable such that larger displacements occur for smaller load increments. This type of instability can manifest itself as a global or local effect. Global instability occurs when the global load-displacement response is characterized by a negative stiffness such as collapse or "snap-through" of structure whereby the structure releases strain energy to maintain equilibrium (Abaqus Analysis User's Manual, 2007). This type of behavior can be analyzed by using the modified Riks's method (also called the arc length method) or by treating the buckling behavior as a dynamic process. Local buckling is characterized by an instability that appears somewhere within the structure as a whole and the strain energy in this local area is "released" by transferring the energy to the neighboring regions (Abaqus Analysis User's Manual, 2007). For the local instabilities sometimes the techniques mentioned for global instabilities may not work. For local buckling the total load may still increase while buckling occurs ("8.11 Unstable Structures", 2007). In this case the problem must be solved with the help of artificial damping (Abaqus Analysis User's Manual, 2007 and "7.4 Performing a Post-Buckling Analysis", 2007). Conceptually, stabilization can be thought of as adding an artificial dashpot to connect the nodes of an element to some reference location which creates a
viscous force under deformation. These viscous forces act to stabilize the structure locally and are of the form

\[ F_v = cM^\star \dot{v} \]  \hspace{1cm} (D.1)

where \( c \) is a calculated damping factor, \( M^\star \) is an artificial mass matrix of unit density, and \( \dot{v} \) is the pseudo velocity of the nodes calculated as the differential displacement divided by the increment in time

\[ \dot{v} = \frac{\Delta u}{\Delta t} \]

(Abaqus Analysis User's Manual, 2007). When local instabilities occur, the local velocities increase, causing some of the strain energy to be dissipated (Abaqus Analysis User's Manual, 2007). The damping factor is calculated at the first increment that stabilization is enacted according to a user-specified dissipated energy fraction. In Abaqus, this energy fraction can be either constant or adaptive (i.e. automatic), with the default constant value being \( 2 \cdot 10^{-4} \) (Abaqus Analysis User's Manual, 2007). The pseudo velocity can be reduced, thereby reducing the stabilization force, by using smaller time increments. Obviously the inclusion of stabilization has little effect on stable elements as their pseudo velocities and stabilizing forces are small relative to physical forces ("8.11 Unstable Structures", 2007). An analysis has arrived at an accurate solution when the ratio of the viscous dissipation energy for the entire model to the total strain energy is less than a "reasonable amount" (Abaqus Analysis User's Manual, 2007). This reasonable amount depends upon the behavior of the particular model being studied and from experience obtained from previous runs of the same model, and
even large dissipation energies could be obtained from a valid model ("8.11 Unstable Structures", 2007).

Stabilization is implemented into an analysis by inserting the stabilization forces into the global force equilibrium equations as

$$\mathbf{P} - \mathbf{F}_I - \mathbf{F}_v = 0$$

(D.2)

where \( \mathbf{P} \) is a vector of applied forces and \( \mathbf{F}_I \) is a vector of the internal (or restoring) forces. Equilibrium is achieved at an iteration of a certain time for at a loading value \( P \) which is incrementally increased from a previous increment if the left-hand side of equation (D.2) is less than specified convergence criteria, not necessarily zero. In other words, the difference between the applied forces and the internal forces, called \( \mathbf{R} \), is compared with the convergence criteria (Figure D.1). Thus the stabilization forces act to promote equilibrium by reducing the overall difference between these two forces of the elements that are experiencing local instability.

![Figure D.1 Schematic of force-displacement diagram at two iterations, a and b, with (a) showing the initial iteration and the difference between forces to determine convergence and (b) showing the second iteration with a cut in the time increment in order to reduce the difference in forces (Courtesy of Abaqus Analysis User's Manual, 2007).](image)
For the simulations of the Si-PDMS anode system, local buckling occurs as the Si film wrinkles. Convergence beyond the initiation of buckling cannot be achieved using the standard nonlinear solution techniques. Thus stabilization is employed in order to overcome the instabilities. The amount of stabilization a user must specify is problem dependent and usually requires some trial and error to obtain a converged solution that uses the appropriate amount of stabilization. Too much dissipation energy will cause distortion and too little will not control the instability (Abaqus Analysis User's Manual). Thus the Si-PDMS model is subjected to test cases whereby the amount of the specified dissipated energy fraction is varied in order to determine the optimal value. Several analyses are performed (Table D.1) beyond the critical 5% strain as they normally would until they begin to diverge at approximately 10% strain. The Si structure is unstable at this point because of the propagation of waves down its length. Stabilization (at varying magnitudes) is implemented at 10% strain and the ratio of the dissipation energy to the total strain energy is compared between these cases in order to evaluate which level of stabilization will be appropriate.

Table D.1

<table>
<thead>
<tr>
<th>Case</th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
<th>E</th>
<th>F</th>
<th>H</th>
<th>J</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dissipation Energy Fraction</td>
<td>(1 \cdot 10^{-3})</td>
<td>(4 \cdot 10^{-4})</td>
<td>(2 \cdot 10^{-4})</td>
<td>(1 \cdot 10^{-4})</td>
<td>(4 \cdot 10^{-5})</td>
<td>(1 \cdot 10^{-5})</td>
<td>(5 \cdot 10^{-6})</td>
<td>(1 \cdot 10^{-6})</td>
</tr>
</tbody>
</table>

It was found that the Cases A-E had a significant amount of the total strain energy being dissipated (Figure D.2). The resulting deformed model for these
cases experienced distortion of the PDMS elements near the buckled Si thin film; however the significance of this distortion decreased as the dissipated energy fraction is reduced. Dissipation as specified by Case F and Case H produced very smooth, undistorted morphologies. The ratio of dissipation energy to the total strain energy is less than 5% for Case F and less than 3% for Case H. The final case, Case J, performed well at lower strains, but it was unable control the instability effectively, with the ratio of energies beginning to increase rapidly just 25% strain (Figure D.2) and growing significantly beyond this strain. Thus the smallest amount of stabilization to achieve a converged result is used (Case H) for all subsequent analyses in order to analyze the behavior of the Si-PDMS anode system beyond buckling. It should be noted that the convergence test as previously discussed were carried to 25% strain using the dissipated energy level of Case H and these stabilization trials used the meshing strategy of Case 3.
Displayed in this appendix are sample Matlab scripts that will generate planar simulation input files for submission in Abaqus. This script allows the user to easily define meshing parameters for the analysis. The mesh of the silicon is a regular pattern of planar elements that can be easily coded using for-loops. The sometimes irregular mesh of the partitioned substrate cannot be coded easily, thus the generation of nodes, elements, and analysis sets/surfaces must be created using Abaqus CAE, copied from the generated input file, and then pasted into the complete. The user must be cautious to mesh the substrate appropriately to match with the generate Si ribbon at the interface.

The generated input files can be easily altered manually in order to perform the analyses for the charge rate and the plasticity analyses by adjusting the material properties appropriately.

E.1 Planar Analysis: Linear Buckling Matlab Script

```matlab
% Creates Linear Plane Elements for Film for Linear Buckling Analysis
% For an even number of layers only

clear all;
close all;
c
c
% MODEL PARAMETERS
w = 500;           %Model width
h = 0.1;           %Film thickness
hsub = 1250;       %Substrate thickness
D = 5000;          %Number of divisions (elements)
LE = 4;            %Number of element layers (MUST BE EVEN IN ORDER TO GET CORRECT NODE PLACEMENT)
LN = LE+1;         %Number of node layers
ce = 0;            %Element layer counter
cn = 0;            %Node layer counter
mode = 40;         %Number of modes to extract

% FILM ELEMENT ASPECT RATIO
Dx = w/D;
Dy = h/LE;
alpha = Dx/Dy;
```
% MATERIAL PROPERTIES
bot_factor = 1.0; % Percentage of Bulk Si CTE for bottom layer
CTE_bulk = 2.6e-6; % CTE of bulk Si

CTE_film = zeros(ce); % Vector of CTE coefficients
CTE_film(1) = CTE_bulk; % Define the first layer CTE to be bulk Si
inc = (bot_factor-1)/(LE-1); % Increment for linear interpolation of layer CTE
for ce=2:LE
    CTE_film(ce) = CTE_bulk+(ce-1)*inc*CTE_bulk;
end

% OUTPUT FILE SPECIFICATION
fid = fopen('buckle_out.txt','w');

% INPUT FILE GENERATION - HEADING
fprintf(fid,'%s
','*HEADING');
fprintf(fid,'%s
',[' LINEAR BUCKLING: ' num2str(LE) ' LAYER, PE (' num2str(h*1000) ' nm)']);
fprintf(fid,'%s
',['** JOB NAME: BUCKLE_2D_' num2str(LE) 'L MODEL NAME: BUCKLE_MODEL']);
fprintf(fid,'%s
','*Preprint, echo=NO, model=NO, history=NO, contact=NO');
fprintf(fid,'%s
','**');

% INPUT FILE GENERATION - PART DEFINITION
fprintf(fid,'%s
','** PARTS');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*PART, NAME=FILM_PART');
fprintf(fid,'%s
','*END PART');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*PART, NAME=SUB_PART');
fprintf(fid,'%s
','*End Part');
fprintf(fid,'%s
','**');

% INPUT FILE GENERATION - ASSEMBLY
fprintf(fid,'%s
','** ASSEMBLY');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*ASSEMBLY, NAME=ASSEMBLY');
fprintf(fid,'%s
','**');

% INPUT FILE GENERATION - SUBSTRATE INSTNACE
fprintf(fid,'%s
','*INSTANCE, NAME=SUB_INST, PART=SUB_PART');

fprintf(fid,'%s
',' ');fprintf(fid,'%s
',' ');fprintf(fid,'%s
','---------- INSERT SUBSTRATE NODES & ELEMENTS HERE ----------');
fprintf(fid,'%s
',' ');fprintf(fid,'%s
',' ');fprintf(fid,'%s
','');

% INPUT FILE GENERATION - FILM NODES/ELEMENTS
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*INSTANCE, NAME=FILM_INST, PART=FILM_PART');
fprintf(fid,'%s
',['        0,       ' num2str(hsub/2+2*h/LE) ',           0']);
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** FILM NODE GENERATION');
fprintf(fid,'%s
','**');
for cn = 1:LN
    fprintf(fid,’%s
’,’*NODE’);
    fprintf(fid,’%s’,[num2str((cn-1)*D+cn) ‘, ‘ num2str(-1/2*w) ‘, ‘ num2str(1/2*h-1/LE*(cn-1)*h)]);
    fprintf(fid,’%s
’,[num2str(cn*D+cn) ‘, ‘ num2str(1/2*w) ‘, ‘ num2str(1/2*h-1/LE*(cn-1)*h)]);
    fprintf(fid,’%s
’,’*NGEN’);
    fprintf(fid,’%s
’,[num2str((cn-1)*D+cn) ‘, ‘ num2str(cn*D+cn) ‘, ‘ ‘1’]);
end

fprintf(fid,’%s
’,’**’);
fprintf(fid,’%s
’,’** FILM ELEMENT GENERATION’);
fprintf(fid,’%s
’,’**’);
for ce = 1:LE
    fprintf(fid,’%s
’,’*ELEMENT, TYPE=CPS4R’);
    fprintf(fid,’%s
’,[num2str((ce-1)*D+1) ‘, ‘ num2str((ce-1)*D+ce+1) ‘, ‘ num2str((ce-1)*D+ce) ‘, ‘ num2str(ce*D+ce+1) ‘, ‘ num2str(ce*D+ce+2)]);
    fprintf(fid,’%s
’,’*ELGEN’);
    fprintf(fid,’%s
’,[num2str((ce-1)*D+1) ‘, ‘ num2str(D) ‘, 1, 1’]);
end

fprintf(fid,’%s
’,’**’);
fprintf(fid,’%s
’,’** NODE SETS’);
fprintf(fid,’%s
’,’**’);
for cn = 1:(LN-1)
    fprintf(fid,’%s
’,’*NSET, NSET=LAYER_' num2str(cn) '_NODE, GENERATE’);
    fprintf(fid,’%s
’,[num2str((cn-1)*D+cn) ‘, ‘ num2str(cn*D+cn) ‘, ‘ ‘1’]);
    fprintf(fid,’%s
’,[num2str((cn)*D+cn+1) ‘, ‘ num2str((cn+1)*D+cn+1) ‘, ‘ ‘1’]);
end

fprintf(fid,’%s
’,’**’);
fprintf(fid,’%s
’,’** ELEMENT SETS’);
fprintf(fid,’%s
’,’**’);
for ce = 1:LE
    fprintf(fid,’%s
’,’*ELSET, ELSET=LAYER_' num2str(ce) '_ELEM, GENERATE’);
    fprintf(fid,’%s
’,[num2str((ce-1)*D+1) ‘, ‘ num2str(ce*D) ‘, ‘ ‘1’]);
end

fprintf(fid,’%s
’,’**’);
fprintf(fid,’%s
’,’** ASSIGN SECTIONS’);
fprintf(fid,’%s
’,’**’);
for ce = 1:LE

    fprintf(fid,_inches,'%s
',['*SOLID SECTION, ELSET=LAYER_ ' num2str(ce) ' _ELEM, MATERIAL=LAYER_ ' num2str(ce) ' _PROP']);
    fprintf(fid,_inches,'%s
',['*END INSTANCE']);

end

fprintf(fid,setVisible,'**');
fprintf(fid,setVisible,'*END INSTANCE');
fprintf(fid,setVisible,'**');

% INPUT FILE GENERATION - ANALYSIS SETS
fprintf(fid,setVisible,'**');
fprintf(fid,setVisible,'** SETS FOR ANALYSIS');
fprintf(fid,setVisible,'**');
fprintf(fid,setVisible,'** BASE BC');
fprintf(fid,setVisible,'*NSET, NSET=BASE_NODE, INSTANCE=Sub_Inst');
fprintf(fid,setVisible,'---------- REQUIRES MANUAL INPUT ----------');
fprintf(fid,setVisible,'*ELSET, ELSET=BASE_ELEM, INSTANCE=SUB_INST');
fprintf(fid,setVisible,'---------- REQUIRES MANUAL INPUT ----------');
fprintf(fid,setVisible,'**');
fprintf(fid,setVisible,'** TIE SURFACES');
fprintf(fid,setVisible,'**');
fprintf(fid,setVisible,'*ELSET, ELSET=FILM_TIE_ELEM, INSTANCE=FILM_INST, GENERATE');
fprintf(fid,setVisible,_inches,[num2str((LE-1)*D+1) ', ' num2str(LE*D) ', ' '1']);
fprintf(fid,setVisible,'*SURFACE, TYPE=ELEMENT, NAME=FILM_TIE_SURF');
fprintf(fid,setVisible,人居环境,_inches,'FILM_TIE_ELEM, S3');
fprintf(fid,setVisible,'*ELSET, ELSET=SUB_TIE_ELEM, INSTANCE=SUB_INST, GENERATE');
fprintf(fid,setVisible,人居环境,_inches,'---------- REQUIRES MANUAL INPUT ----------');
fprintf(fid,setVisible,'*SURFACE, TYPE=ELEMENT, NAME=SUB_TIE_SURF');
fprintf(fid,setVisible,'Sub_Tie_Elem, S3');
fprintf(fid,setVisible,人居环境);"}

for ce = 1:LE

    fprintf(fid,_inches,['*ELSET, ELSET=LAYER_ ' num2str(ce) ' _LEFT_LOAD_ELEM, INSTANCE=FILM_INST']);
    fprintf(fid,_inches,num2str((ce-1)*D+1));
    fprintf(fid,_inches,['*SURFACE, TYPE=ELEMENT, NAME=LAYER_ ' num2str(ce) ' _LEFT_LOAD_ELEM', 'LEFT_LOAD_ELEM, S2']);

end

fprintf(fid,setVisible,'**');
fprintf(fid,setVisible,'** RIGHT LOAD SURFACES (S4)');
fprintf(fid,setVisible,'**');
for ce = 1:LE
  fprintf(fid,'%s
','[*ELSET, ELSET=LAYER_' num2str(ce) ' _RIGHT_LOAD_ELEM,
    INSTANCE=FILM_INST]
  );
  fprintf(fid,'%s
',num2str(ce*D));
  fprintf(fid,'%s
','[*SURFACE, TYPE=ELEMENT, NAME=LAYER_' num2str(ce) ' _RIGHT_LOAD_SURF]
  );
  fprintf(fid,'%s
',
    'LAYER_' num2str(ce) ' _RIGHT_LOAD_ELEM, S4'
  );
end

%INPUT FILE GENERATION - BONDED CONSTRAINT
fprintf(fid,'%s
','** Constraints: FILM_SUB_BOND
');
fprintf(fid,'%s
','*TIE, NAME=FILM_SUB_BOND, ADJUST=YES');
fprintf(fid,'%s
','SUB_TIE_SURF, FILM_TIE_SURF');
fprintf(fid,'%s
','*End Assembly');

%INPUT FILE GENERATION - MATERIALS
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** MATERIALS');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*MATERIAL, NAME=SUB_PROP');
fprintf(fid,'%s
','*ELASTIC');
fprintf(fid,'%s
','2., 0.49');
fprintf(fid,'%s
','*EXPANSION');
fprintf(fid,'%s
','0.00034');
for ce = 1:LE
  fprintf(fid,'%s
',
    '*MATERIAL, NAME=LAYER_' num2str(ce) ' _PROP
  ');  fprintf(fid,'%s
','*ELASTIC
  ');  fprintf(fid,'%s
','130000, 0.3
  ');  fprintf(fid,'%s
','*EXPANSION
  ');  fprintf(fid,'%s
',num2str(CTE_film(ce))
  );
end

%INPUT FILE GENERATION - LOAD STEP (LINEAR BUCKLING)
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** STEP: BUCKLE_STEP
');
fprintf(fid,'%s
','*STEP, NAME=BUCKLE_STEP, PERTURBATION
');
fprintf(fid,'%s
','*BUCKLE, EIGENSOLVER=LANCZOS
');
fprintf(fid,'%s
','**
');
%INPUT FILE GENERATION - BOUNDARY CONDITIONS
fprintf(fid,'%s
',"** BOUNDARY CONDITIONS");
fprintf(fid,'%s
',"**");
fprintf(fid,'%s
',"** NAME: BASE_BC TYPE: DISPLACEMENT/ROTATION");
fprintf(fid,'%s
',"**BOUNDARY");
fprintf(fid,'%s
',"BASE_NODE, 1, 1");
fprintf(fid,'%s
',"BASE_NODE, 2, 2");

%INPUT FILE GENERATION - PRESSURE LOADS
fprintf(fid,'%s
',"**");
fprintf(fid,'%s
',"** LOADS");
fprintf(fid,'%s
',"**");
for ce = 1:LE
   fprintf(fid,'%s
',"** NAME: LAYER_' num2str(ce) '_LEFT_LOAD TYPE: PRESSURE");
   fprintf(fid,'%s
',"*DSLOAD");
   fprintf(fid,'%s
',"LAYER_' num2str(ce) '_LEFT_LOAD_SURF, P, 1");
   fprintf(fid,'%s
',"** NAME: LAYER_' num2str(ce) '_RIGHT_LOAD TYPE: PRESSURE");
   fprintf(fid,'%s
',"*DSLOAD");
   fprintf(fid,'%s
',"LAYER_' num2str(ce) '_RIGHT_LOAD_SURF, P, 1");
end

%INPUT FILE GENERATION - OUTPUT REQUESTS
fprintf(fid,'%s
',"**");
fprintf(fid,'%s
',"** OUTPUT REQUESTS");
fprintf(fid,'%s
',"**");
fprintf(fid,'%s
',"*RESTART, WRITE, FREQUENCY=0");
fprintf(fid,'%s
',"**");
fprintf(fid,'%s
',"*NODE PRINT, GLOBAL=YES");
fprintf(fid,'%s
',"U");
fprintf(fid,'%s
',"*NODE FILE");
fprintf(fid,'%s
',"U,COORD");

%INPUT FILE GENERATION - END STEP
fprintf(fid,'%s
',"**");
fprintf(fid,'%s
',"*END STEP");
fprintf(fid,'%s
',"**");

%DISPLAY THE ASPECT RATIO
display('')
display('')
display('The Aspect Ratio of the Film Elements is:')
display(num2str(alpha))
E.2 Planar Analysis: Post-buckling Matlab Script

% Creates Linear Plane Elements for the Film for Post-Buckling Analysis
% For an even number of layers only

clear all;
close all;
clc

% MODEL PARAMETERS
w = 500;          %Model width
h = 0.1;          %Film thickness
hsub = 1250;      %Substrate thickness
D = 5000;         %Number of divisions (elements)
LE = 4;           %Number of element layers (MUST BE EVEN IN ORDER TO GET CORRECT
                  NODE PLACEMENT)
LN = LE+1;        %Number of node layers
ce = 0;           %Element layer counter
cn = 0;           %Node layer counter
mode = 40;        %Number of modes to extract

% FILM ELEMENT ASPECT RATIO
Dx = w/D;
Dy = h/LE;
alpha = Dx/Dy;

% LOAD STEP PARAMETERS
init_step = 0.1;            %Initial step value
final_step = 15;            %Final step value (i.e. the specified thermal strain on top layer)
min_step = 0.0001;          %Minimum time step value
max_step = 0.2;             %Maximum time step value

% MATERIAL PROPERTIES
bot_factor = 1.0;               %Percentage of Bulk Si CTE for bottom layer
CTE_bulk = 2.6e-6;              %CTE of bulk Si

CTE_film = zeros(ce);           %Vector of CTE coefficients
CTE_film(1) = CTE_bulk;         %Define the first layer CTE to be bulk Si
inc = (bot_factor-1)/(LE-1);    %Increment for linear interpolation of layer CTE
for ce=2:LE
    CTE_film(ce) = CTE_bulk+(ce-1)*inc*CTE_bulk;
end

%OUTPUT FILE SPECIFICATION
fid = fopen('post_out.txt','w');

fprintf(fid,'%s
','*HEADING');
fprintf(fid,'%s
',' POST-BUCKLING: NR, ' num2str(final_step) '% STRAIN, ' num2str(imp_factor*100) '% IMP, ' num2str(LE) ' LAYER, PE (' num2str(h*1000) 'nm)'
');
fprintf(fid,'%s
','** JOB NAME: POST_2D_' num2str(LE) 'L MODEL NAME: POST_MODEL');
fprintf(fid,'%s
','Preprint, echo=NO, model=NO, history=NO, contact=NO');
fprintf(fid,'%s
','**');

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%INPUT FILE GENERATION - HEADING
fprintf(fid,'#%s
','*HEADING');
fprintf(fid,'#%s
',[' LINEAR BUCKLING: ' num2str(LE) ' LAYER, PE (' num2str(h*1000) 'nm)']);
fprintf(fid,'#%s
',['** JOB NAME: BUCKLE_2D_' num2str(LE) 'L MODEL NAME: BUCKLE_MODEL']);
fprintf(fid,'#%s
','*Preprint, echo=NO, model=NO, history=NO, contact=NO');
fprintf(fid,'#%s
','**');

%INPUT FILE GENERATION - PART DEFINITION
fprintf(fid,'#%s
','** PARTS');
fprintf(fid,'#%s
','**');
fprintf(fid,'#%s
','*PART, NAME=FILM_PART');
fprintf(fid,'#%s
','*END PART');
fprintf(fid,'#%s
','**');
fprintf(fid,'#%s
','*PART, NAME=SUB_PART');
fprintf(fid,'#%s
','*End Part');
fprintf(fid,'#%s
','**');

%INPUT FILE GENERATION - ASSEMBLY
fprintf(fid,'#%s
','** ASSEMBLY');
fprintf(fid,'#%s
','**');
fprintf(fid,'#%s
','*ASSEMBLY, NAME=ASSEMBLY');
fprintf(fid,'#%s
','**');

%INPUT FILE GENERATION - SUBSTRATE INSTNACE
fprintf(fid,'#%s
','*INSTANCE, NAME=SUB_INST, PART=SUB_PART');
fprintf(fid,'#%s
','');
fprintf(fid,'#%s
','');
fprintf(fid,'#%s
','---------- INSERT SUBSTRATE NODES & ELEMENTS HERE ----------');
fprintf(fid,'#%s
','');
fprintf(fid,'#%s
','');

%INPUT FILE GENERATION - FILM NODES/ELEMENTS
fprintf(fid,'#%s
','**');
fprintf(fid,'#%s
','*INSTANCE, NAME=FILM_INST, PART=FILM_PART');
fprintf(fid,'#%s
',[num2str((cn-1)*D+cn) ', ' num2str(-1/2*w) ', ' num2str(1/2*h-1/LE*(cn-1)*h)']);
fprintf(fid,'#%s
',[num2str(cn*D+cn) ', ' num2str(1/2*w) ', ' num2str(1/2*h-1/LE*(cn-1)*h)']);
fprintf(fid,'#%s
','*NGEN');
fprintf(fid,'#%s
',[num2str((cn-1)*D+cn) ', ' num2str(cn*D+cn) ', ' '1'']);
end

for cn = 1:LN
fprintf(fid,'#%s
','*NODE');
fprintf(fid,'#%s
',[num2str((cn-1)*D+cn) ', ' num2str(-1/2*w) ', ' num2str(1/2*h-1/LE*(cn-1)*h)']);
fprintf(fid,'#%s
',[num2str(cn*D+cn) ', ' num2str(1/2*w) ', ' num2str(1/2*h-1/LE*(cn-1)*h)']);
fprintf(fid,'#%s
','*NGEN');
fprintf(fid,'#%s
',[num2str((cn-1)*D+cn) ', ' num2str(cn*D+cn) ', ' '1'']);
end
fprintf(fid,'%s
','** FILM ELEMENT GENERATION');

for ce = 1:LE

    fprintf(fid,'%s
','*ELEMENT, TYPE=CPS4R');
    fprintf(fid,'%s
',[num2str((ce-1)*D+1) ', ' num2str((ce-1)*D+ce+1) ', ' num2str((ce-1)*D+ce) ', ' num2str(ce*D+ce+1) ', ' num2str(ce*D+ce+2)]);
    fprintf(fid,'%s
','*ELGEN');
    fprintf(fid,'%s
',[num2str((ce-1)*D+1) ', ' num2str(D) ', 1, 1']);

end

fprintf(fid,'%s
','** NODE SETS');

for cn = 1:(LN-1)

    fprintf(fid,'%s
','*NSET, NSET=LAYER_' num2str(cn) '_NODE, GENERATE');
    fprintf(fid,'%s
',[num2str((cn-1)*D+cn) ', ' num2str(cn*D+cn) ', ' '1']);
    fprintf(fid,'%s
',[num2str((cn)*D+cn+1) ', ' num2str((cn+1)*D+cn+1) ', ' '1']);

end

fprintf(fid,'%s
','** ELEMENT SETS');

for ce = 1:LE

    fprintf(fid,'%s
','*ELSET, ELSET=LAYER_' num2str(ce) '_ELEM, GENERATE');
    fprintf(fid,'%s
',[num2str((ce-1)*D+1) ', ' num2str(ce*D) ', ' '1']);

end

fprintf(fid,'%s
','** ASSIGN SECTIONS');

for ce = 1:LE

    fprintf(fid,'%s
','*SOLID SECTION, ELSET=LAYER_' num2str(ce) '_ELEM, MATERIAL=LAYER_' num2str(ce) '_PROP');
    fprintf(fid,'%s
','1');

end

fprintf(fid,'%s
','*END INSTANCE');

fprintf(fid,'%s
','**');
%INPUT FILE GENERATION - ANALYSIS SETS
fprintf(fid,'%s
','**
');
fprintf(fid,'%s
','** SETS FOR ANALYSIS');
fprintf(fid,'%s
','**
');
fprintf(fid,'%s
','** BASE BC');
fprintf(fid,'%s
','**
');
fprintf(fid,'%s
','NSET, NSET=BASE_NODE, INSTANCE=Sub_Inst');
fprintf(fid,'%s
',',---------- REQUIRES MANUAL INPUT ----------');
fprintf(fid,'%s
','*ELSET, ELSET=BASE_ELEM, INSTANCE=SUB_INST, GENERATE');
fprintf(fid,'%s
',',---------- REQUIRES MANUAL INPUT ----------');
fprintf(fid,'%s
','**
');
fprintf(fid,'%s
','** TIE SURFACES');
fprintf(fid,'%s
','**
');
fprintf(fid,'%s
','ELSET, ELSET=FILM_TIE_ELEM, INSTANCE=FILM_INST, GENERATE');
fprintf(fid,'%s
',',num2str((LE-1)*D+1) ', ,num2str(LE*D) ', ,1']);
fprintf(fid,'%s
','SURFACE, TYPE=ELEMENT, NAME=FILM_TIE_SURF');
fprintf(fid,'%s
','FILM_TIE_ELEM, S3');
fprintf(fid,'%s
','*ELSET, ELSET=SUB_TIE_ELEM, INSTANCE=SUB_INST, GENERATE');
fprintf(fid,'%s
',',---------- REQUIRES MANUAL INPUT ----------');
fprintf(fid,'%s
','SURFACE, TYPE=ELEMENT, NAME=SUB_TIE_SURF');
fprintf(fid,'%s
','Sub_Tie_Elem, S3');
fprintf(fid,'%s
','** TEMPERATURE LOAD SETS');
fprintf(fid,'%s
','**
');
fprintf(fid,'%s
','NSET, NSET=FILM_NODE, INSTANCE=FILM_INST, GENERATE');
fprintf(fid,'%s
',',num2str(D+1) ', ,num2str(D));
fprintf(fid,'%s
','ELSET, ELSET=FILM_ELEM, INSTANCE=FILM_INST, GENERATE');
fprintf(fid,'%s
',',1, ,num2str(D*D+1));
fprintf(fid,'%s
','**
');
fprintf(fid,'%s
','** BONDED CONSTRAINT');
fprintf(fid,'%s
','**
');
fprintf(fid,'%s
','CONSTR: FILM_SUB_BOND');
fprintf(fid,'%s
','TIE, NAME=FILM_SUB_BOND, ADJUST=YES');
fprintf(fid,'%s
','SUB_TIE_SURF, FILM_TIE_SURF');
fprintf(fid,'%s
','End Assembly');
fprintf(fid,'%s
','**
');
fprintf(fid,'%s
','** MATERIALS');
fprintf(fid,'%s
','**
');
fprintf(fid,'%s
','MATERIAL, NAME=SUB_PROP');
fprintf(fid,'%s
','ELASTIC');
fprintf(fid,'%s
',',2, ,0.49
');
fprintf(fid,'%s
','EXPANSION');
fprintf(fid,'%s
',',0.00034
');
fprintf(fid,'%s
','');

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for ce = 1:LE
    fprintf(fid,'%s
', 
        ['*MATERIAL, NAME=LAYER_' num2str(ce) '_PROP']);
    fprintf(fid,'%s
', '*ELASTIC');
    fprintf(fid,'%s
', ['130000, 0.3']);
    fprintf(fid,'%s
', '*EXPANSION');
    fprintf(fid,'%s
', num2str(CTE_film(ce)));
end

%INPUT FILE GENERATION - LOAD STEP (POST-BUCKLING)
fprintf(fid,'%s
','** ----------------------------------------------------------------');
fprintf(fid,'%s
','**');

%INPUT FILE GENERATION - BOUNDARY CONDITIONS
fprintf(fid,'%s
','** BOUNDARY CONDITIONS');
fprintf(fid,'%s
','** NAME: BASE_BC TYPE: DISPLACEMENT/ROTATION');
fprintf(fid,'%s
','*BOUNDARY');
fprintf(fid,'%s
','BASE_NODE, 1, 1');
fprintf(fid,'%s
','BASE_NODE, 2, 2');
fprintf(fid,'%s
','**');

%INPUT FILE GENERATION - LOAD STEP OPTIONS
fprintf(fid,'%s
','** STEP: Step-1');
fprintf(fid,'%s
','*STEP, NLGEOM');
fprintf(fid,'%s
', [num2str(init_step) ', ' num2str(final_step) ', ' num2str(min_step) ', ' num2str(max_step)]);
fprintf(fid,'%s
','**');

%INPUT FILE GENERATION - TEMPERATURE LOAD
fprintf(fid,'%s
','** LOADS');
fprintf(fid,'%s
','** NAME: EIGENSTRAIN (THERMAL) TYPE: TEMPERATURE');
fprintf(fid,'%s
','*TEMPERATURE');
fprintf(fid,'%s
', ['FILM_NODE, ' num2str(round(final_step*0.01/CTE_bulk))]);
%INPUT FILE GENERATION - OUTPUT REQUESTS
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** OUTPUT REQUESTS');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*RESTART, WRITE, FREQUENCY=1');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** FIELD OUTPUT: OUT_REQUEST');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*OUTPUT, FIELD');
fprintf(fid,'%s
','*NODE OUTPUT');
fprintf(fid,'%s
','NT, U');
fprintf(fid,'%s
','*ELEMENT OUTPUT, DIRECTIONS=YES');
fprintf(fid,'%s
','TEMP, S, E, LE, THE, TEMP');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** HISTORY OUTPUT: OUT_REQUEST');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*OUTPUT, HISTORY');
fprintf(fid,'%s
','*ENERGY OUTPUT');
fprintf(fid,'%s
','ETOTAL, ALLSE, ALLSD, ALLIE, ALLAE');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** PRINT RESULTS');
fprintf(fid,'%s
','*EL PRINT, ELSET=TOP_ELEM, FREQUENCY=5');
fprintf(fid,'%s
',' S,E, TEMP');
fprintf(fid,'%s
','*EL FILE, FREQUENCY=5');
fprintf(fid,'%s
',' S,E, TEMP');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** PRINT NODAL RESULTS');
fprintf(fid,'%s
','*NODE PRINT, NSET=TOP_NODE, FREQUENCY=5');
fprintf(fid,'%s
',' U, NT');
fprintf(fid,'%s
','*NODE FILE, FREQUENCY=5');
fprintf(fid,'%s
',' U, NT');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*END STEP');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** DISPLAY THE ASPECT RATIO
display(" ")
display(" ")
display('The Aspect Ratio of the Film Elements is:')
display(num2str(alpha))
APPENDIX F

ABAQUS THREE-DIMENSIONAL SAMPLE INPUT SCRIPT
Displayed in this appendix are sample Matlab scripts that will generate three-dimensional simulation input files for submission in Abaqus. This script allows the user to easily define meshing parameters for the analysis. The mesh of the silicon is a regular pattern of brick elements that can be easily coded using for-loops. The tetrahedral mesh of the substrate cannot be coded easily, thus the generation of nodes, elements, and analysis sets/surfaces must be created using Abaqus CAE, copied from the generated input file, and then pasted into the complete. The user must be cautious to mesh the substrate appropriately to match with the generate Si ribbon at the interface.

F.1 3-D Analysis: Linear Buckling Matlab Script

% Creates Linear Brick Elements for 3D Ribbon for Linear Buckling Analysis
% For an any number of layers (thickness and width) only
% Nodal Positions will work out MUCH BETTER if you use an even number of layers

clear all;
close all;
cle

% MODEL PARAMETERS
HS = 500;           %Substrate thickness [micron]
L = 200;            %Ribbon Length [micron]
W = 1;              %Ribbon width [micron] - Actually half the width due to the symmetry boundary condition
H = 0.1;            %Ribbon thickness [micron]
dze = 750;          %Number of element divisions down ribbon length (Ensure this matches up with mesh of substrate)
dye = 2;            %Number of element divisions through ribbon thickness (EVEN NUMBER IS ADVISED)
dxe = 6;            %Number of element divisions down ribbon width (EVEN NUMBER IS ADVISED)
dzn = dze+1;        %Number of node layers down ribbon length
dyn = dye+1;        %Number of node layers through ribbon thickness
dx = dxe+1;         %Number of node layers down ribbon width
cy = 0;             %Element layer counter (thickness)
cx = 0;             %Element layer counter (width)
cyn = 0;            %Node layer counter (thickness)
cxn = 0;            %Node layer counter (width)
% FILM ELEMENT ASPECT RATIO
Dz = L/dze;
Dy = H/dye;
Dx = W/dxe;
alpha_xy = Dx/Dy;
alpha_zx = Dz/Dx;
alpha_zy = Dz/Dy;

%OUTPUT FILE SPECIFICATION
fid = fopen('buckle_3d_out.txt','w');

%INPUT FILE SPECIFICATION - HEADING
fprintf(fid,'%s
','*HEADING');
fprintf(fid,'%s
',' LINEAR BUCKLING: X,Y,Z DIV = ' num2str(dxe) ' num2str(dye) num2str(dze) (H*1000 nm THICK)');
fprintf(fid,'%s
','** JOB NAME: Buckle MODEL NAME: Buckle_Model');
fprintf(fid,'%s
','*Preprint, echo=NO, model=NO, history=NO, contact=NO');
fprintf(fid,'%s
','**

%INPUT FILE SPECIFICATION - PART DEFINITION
fprintf(fid,'%s
','** PARTS');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*PART, NAME=BULK_3D');
fprintf(fid,'%s
','*END PART');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*PART, NAME=INT_3D');
fprintf(fid,'%s
','*END PART');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*PART, NAME=RIB_3D');
fprintf(fid,'%s
','*END PART');
fprintf(fid,'%s
','**');

%INPUT FILE SPECIFICATION - ASSEMBLY
fprintf(fid,'%s
','** ASSEMBLY');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*ASSEMBLY, NAME=ASSEMBLY');
fprintf(fid,'%s
','**

%INPUT FILE SPECIFICATION - RIBBON NODES/ELEMENTS
fprintf(fid,'%s
','*INSTANCE, NAME=BULK_3D_INST, PART=BULK_3D');
fprintf(fid,'%s
','*Nset, nset=_PickedSet2, internal, generate');
fprintf(fid,'%s
','     1,  44804,      1');
fprintf(fid,'%s
','*Elset, elset=_PickedSet2, internal, generate');
fprintf(fid,'%s
','      1,  202524,       1');
fprintf(fid,'%s
','** Section: Sub_Sec');
fprintf(fid,'%s
','*Solid Section, elset=_PickedSet2, material=Sub_Prop');
fprintf(fid,'%s
','1.,');
fprintf(fid,'%s
','*End Instance');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*INSTANCE, NAME=INT_3D_INST, PART=INT_3D');
fprintf(fid,'%s
', '4.5, 0., 0.);
fprintf(fid,'%s
');
fprintf(fid,'%s
','---------------- INSERT SUBSTRATE NODES & ELEMENTS HERE ----------------');
fprintf(fid,'%s
');
fprintf(fid,'%s
','*Nset, nset=_PickedSet2, internal, generate');
fprintf(fid,'%s
','1, 99883, 1');
fprintf(fid,'%s
','*Elset, elset=_PickedSet2, internal, generate');
fprintf(fid,'%s
','1, 81000, 1');
fprintf(fid,'%s
','** Section: Sub_Sec');
fprintf(fid,'%s
','*Solid Section, elset=_PickedSet2, material=Sub_Prop');
fprintf(fid,'%s
','1.,');
fprintf(fid,'%s
','*End Instance');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*INSTANCE, NAME=RIB_3D_INST, PART=RIB_3D');
fprintf(fid,'%s
',[num2str(HS), ' 0, 0']);
fprintf(fid,'%s
');
fprintf(fid,'%s
','** RIBBON NODE GENERATION');
fprintf(fid,'%s
');
for cyn = 1:dyn
    for cxn = 1:dxn
        fprintf(fid,'%s
','*NODE');
        fprintf(fid,'%s
',[num2str((cyn-1)*dxn*dzn+(cxn-1)*dze+cxn) ', ' num2str(W-(cxn-1)/dxe*W) ', ' num2str(H-(cyn-1)/dye*H) ', ' 0]);
        fprintf(fid,'%s
',[num2str((cyn-1)*dxn*dzn+(cxn-1)*dze+cxn) ', ' num2str((cyn-1)*dxn*dzn+(cxn-1)*dze+cxn) ', ' 1]);
    end
end

fprintf(fid,'%s
','** RIBBON ELEMENT GENERATION');
fprintf(fid,'%s
');
for cye = 1:dye
    for cxe = 1:dxe
        fprintf(fid,'%s
','*ELEMENT, TYPE=C3D8R');
        fprintf(fid,'%s
',[num2str((cxe-1)*dze+(cye-1)*dxn*dzn) ', ' num2str((cxe-1)*dze+cxe+(cye-1)*dxn*dzn) ', ...
num2str((cxe-1)*dze+cxe+(cye-1)*dxn*dzn+1) ', ' num2str((cxe-1)*dze+cxe+(cye-1)*dxn*dzn+2) ', ...
num2str(cxe*dze+cxe+(cye-1)*dxn*dzn+1) ', ' num2str(cxe*dze+cxe+(cye-1)*dxn*dzn+2) ', ...
num2str(cxe*dze+cxe+(cye-1)*dxn*dzn+2) ']);
    end
end
fprintf(fid,'%s
','*ELGEN');
fprintf(fid,'%s
',[num2str((cxe-1)*dze+(cye-1)*dxe*dze+1) ', ' num2str(dze) ', ' num2str(1) ',
1']);
end
end

fprintf(fid,'%s
','*NSET, NSET=RIB_SET, INSTANCE=RIB_3D_INST, INTERNAL,
GENERATE');
fprintf(fid,'%s
',[num2str(1) ', ' num2str(dxn*dyn*dzn) ', ' num2str(1) ]);  
fprintf(fid,'%s
','*ELSET, ELSET=RIB_SET, INSTANCE=RIB_3D_INST, INTERNAL,
GENERATE');
fprintf(fid,'%s
',[num2str(1) ', ' num2str(dxe*dye*dze) ', ' num2str(1) ]);  

fprintf(fid,'%s
','** SECTION: REB_SEC');
fprintf(fid,'%s
','*SOLID SECTION, ELSET=RIB_SET, MATERIAL=RIB_PROP');
fprintf(fid,'%s
','1');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*END INSTANCE');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** SETS FOR ANALYSIS');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** SYMMETRY SETS');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','**RIBBON');
fprintf(fid,'%s
','*NSET, NSET=RIB_SYMM_SET, INSTANCE=RIB_3D_INST,
GENERATE');
for cyn = 1:dyn
    fprintf(fid,'%s
',[num2str((cyn-1)*dxn*dzn+(dxn-1)*dze+dxn) ', ' num2str((cyn-1)*dxn*dzn+dxn*dze+dxn) ', ' num2str(1) ]);  
end
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*ELSET, ELSET=RIB_SYMM_SET, INSTANCE=RIB_3D_INST,
GENERATE');
for cye = 1:dye
    fprintf(fid,'%s
',[num2str((dxe-1)*dze+(cye-1)*dxe*dze+1) ', ' num2str(dxe*dze+(cye-1)*dxe*dze) ', ' num2str(1) ]);  
end
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*SOLID SECTION, ELSET=RIB_SET, MATERIAL=RIB_PROP');
fprintf(fid,'%s
','1');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*END INSTANCE');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','---------- INSERT SYMM SETS FOR BULK SUBSTRATE ----------');
fprintf(fid,'%s
','*ELSET, ELSET=SUB_SYMM_SET, INSTANCE=INT_3D_INST, GENERATE');
fprintf(fid,'%s
','---------- INSERT SYMM SETS FOR INTERFACE SUBSTRATE ----------');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** BOUNDARY CONDITION SETS');
fprintf(fid,'%s
','**SUBSTRATE');
fprintf(fid,'%s
','*NSET, NSET=SUB_BASE_SET, INSTANCE=BULK_3D_INST');
fprintf(fid,'%s
','---------- INSERT BASE SETS FOR INTERFACE SUBSTRATE ----------');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** RIBBON NODE & ELEMENT SETS');
fprintf(fid,'%s
','** RIBBON NODE & ELEMENT SETS');
fprintf(fid,'%s
','*NSET, NSET=RIB_SET, INSTANCE=RIB_3D_INST, GENERATE');
fprintf(fid,'%s
','*ELSET, ELSET=RIB_SET, INSTANCE=RIB_3D_INST, GENERATE');
fprintf(fid,'%s
','** PRESSURE LOAD SETS & SURFACES');
fprintf(fid,'%s
','** PRESSURE LOAD SETS & SURFACES');
fprintf(fid,'%s
','*ELSET, ELSET=FRONT_FACE_SET, INSTANCE=RIB_3D_INST, GENERATE');
fprintf(fid,'%s
','*ELSET, ELSET=FRONT_FACE_SET, INSTANCE=RIB_3D_INST, GENERATE');
fprintf(fid,'%s
','** TIE CONSTRAINT SETS & SURFACES');
fprintf(fid,'%s
','** TIE CONSTRAINT SETS & SURFACES');
fprintf(fid,'%s
','---------- INSERT TIE SETS FOR BOTTOM BULK-INTERFACE ----------');
fprintf(fid,'
');
fprintf(fid,'%s
','*Elset, elset=_Bulk_Inter_Bot_Tie_Surf_S2, internal,
instance=BULK_3D_INST');
fprintf(fid,'%s
','*');
fprintf(fid,'%s
','---------- INSERT TIE SETS FOR BOTTOM BULK-INTERFACE ----------');
fprintf(fid,'%s
','*Elset, elset=_Bulk_Inter_Bot_Tie_Surf_S4, internal,
instance=BULK_3D_INST');
fprintf(fid,'%s
','*');
fprintf(fid,'%s
','---------- INSERT TIE SETS FOR BOTTOM BULK-INTERFACE ----------');
fprintf(fid,'%s
','*Elset, elset=_Bulk_Inter_Bot_Tie_Surf_S1, internal,
instance=BULK_3D_INST');
fprintf(fid,'%s
','*');
fprintf(fid,'%s
','---------- INSERT TIE SETS FOR BOTTOM BULK-INTERFACE ----------');
fprintf(fid,'%s
','*Surface, type=ELEMENT, name=Bulk_Inter_Bot_Tie_Surf');
fprintf(fid,'%s
','_Bulk_Inter_Bot_Tie_Surf_S3, S3');
fprintf(fid,'%s
','_Bulk_Inter_Bot_Tie_Surf_S2, S2');
fprintf(fid,'%s
','_Bulk_Inter_Bot_Tie_Surf_S4, S4');
fprintf(fid,'%s
','_Bulk_Inter_Bot_Tie_Surf_S1, S1');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*Elset, elset=_Bulk_Inter_Side_Tie-Surf_S3, internal,
instance=BULK_3D_INST');
fprintf(fid,'%s
','*');
fprintf(fid,'%s
','---------- INSERT TIE SETS FOR BOTTOM BULK-INTERFACE ----------');
fprintf(fid,'%s
','*Elset, elset=_Bulk_Inter_Side_Tie-Surf_S4, internal,
instance=BULK_3D_INST');
fprintf(fid,'%s
','*');
fprintf(fid,'%s
','---------- INSERT TIE SETS FOR BOTTOM BULK-INTERFACE ----------');
fprintf(fid,'%s
','*Elset, elset=_Bulk_Inter_Side_Tie-Surf_S2, internal,
instance=BULK_3D_INST');
fprintf(fid,'%s
','*');
fprintf(fid,'%s
','---------- INSERT TIE SETS FOR BOTTOM BULK-INTERFACE ----------');
fprintf(fid,'%s
','*Elset, elset=_Bulk_Inter_Side_Tie-Surf_S1, internal,
instance=BULK_3D_INST');
fprintf(fid,'%s
','*');
fprintf(fid,'%s
','---------- INSERT TIE SETS FOR BOTTOM BULK-INTERFACE ----------');
fprintf(fid,'%s
','*Surface, type=ELEMENT, name=Bulk_Inter_Side_Tie-Surf');
fprintf(fid,'%s
','_Bulk_Inter_Side_Tie-Surf_S3, S3');
fprintf(fid,'%s
','_Bulk_Inter_Side_Tie-Surf_S4, S4');
fprintf(fid,'%s
','_Bulk_Inter_Side_Tie-Surf_S2, S2');
fprintf(fid,'%s
','_Bulk_Inter_Side_Tie-Surf_S1, S1');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** BULK-INTERFACE: INTERFACE');
fprintf(fid,'%s
','*Elset, elset=_Inter_Bulk_Bot_Tie_Surf_S5, internal,
instance=INT_3D_INST');
fprintf(fid,'%s
','*');
fprintf(fid,'%s
','---------- INSERT TIE SETS FOR BOTTOM BULK-INTERFACE ----------');
fprintf(fid,'%s
','*Surface, type=ELEMENT, name=Inter_Bulk_Bot_Tie_Surf');
fprintf(fid,'%s
','_Inter_Bulk_Bot_Tie_Surf_S5, S5');
fprintf(fid,'%s
','*Elset, elset=_Inter_Bulk_Side_Tie_Surf_S4, internal, instance=INT_3D_INST, generate');
fprintf(fid,'%s
','');
fprintf(fid,'%s
','---------- INSERT TIE SETS FOR BULK-INTERFACE ----------');
fprintf(fid,'%s
','*Surface, type=ELEMENT, name=Inter_Bulk_Side_Tie_Surf');
fprintf(fid,'%s
','_Inter_Bulk_Side_Tie_Surf_S4, S4');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** INTERFACE-RIBBON: INTERFACE');
fprintf(fid,'%s
','*Elset, elset=_Inter_Rib_Tie_Surf_S3, internal, instance=INT_3D_INST');
fprintf(fid,'%s
','');
fprintf(fid,'%s
','---------- INSERT TIE SETS FOR RIBBON-INTERFACE ----------');
fprintf(fid,'%s
','*Surface, type=ELEMENT, name=Inter_Rib_Tie_Surf');
fprintf(fid,'%s
','_Inter_Rib_Tie_Surf_S3, S3');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** INTERFACE-RIBBON: RIBBON');
fprintf(fid,'%s
','*ELSET, ELSET=RIB_INT_TIE_SET, INSTANCE=RIB_3D_INST, GENERATE');
fprintf(fid,'%s
','[num2str((dye-1)*dxe*dze+1), num2str(dxe*dze), num2str(1)];');
fprintf(fid,'%s
','*SURFACE, TYPE=ELEMENT, NAME=Rib_Inter_Tie_Surf');
fprintf(fid,'%s
','RIB_INT_TIE_SET, S5');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** TIE CONSTRAINTS');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** Constraint: Inter_Bulk_Bot_TC');
fprintf(fid,'%s
','*Tie, name=Inter_Bulk_Bot_TC, adjust=yes');
fprintf(fid,'%s
','Bulk_Inter_Bot_Tie_Surf, Inter_Bulk_Bot_Tie_Surf');
fprintf(fid,'%s
','** Constraint: Inter_Bulk_Side_TC');
fprintf(fid,'%s
','*Tie, name=Inter_Bulk_Side_TC, adjust=yes');
fprintf(fid,'%s
','Bulk_Inter_Side_Tie_Surf, Inter_Bulk_Side_Tie_Surf');
fprintf(fid,'%s
','** Constraint: Rib_Inter_TC');
fprintf(fid,'%s
','*Tie, name=Rib_Inter_TC, adjust=yes');
fprintf(fid,'%s
','Inter_Rib_Tie_Surf, Rib_Inter_Tie_Surf');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** END ASSEMBLY');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** MATERIALS');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*Material, name=Rib_Prop');
fprintf(fid,'%s
','*Elastic');
fprintf(fid,'%s
','130000., 0.3');
fprintf(fid,'%s
','*Expansion');
fprintf(fid,'%s
','2.6e-06,');
fprintf(fid,'%s
','*Material, name=Sub_Prop');
fprintf(fid,'%s
','**Elastic');
fprintf(fid,"\%s\n","2., 0.49");
fprintf(fid,"\%s\n","*Expansion");
fprintf(fid,"\%s\n"," 0.00034,");
fprintf(fid,"\%s\n","**");
fprintf(fid,"\%s\n","** ----------------------------------------------------------------");
fprintf(fid,"\%s\n","**");

%INPUT FILE GENERATION - LOAD STEP (LINEAR/STATIC)
fprintf(fid,"\%s\n","** STEP: Buckle_Step");
fprintf(fid,"\%s\n","**");
fprintf(fid,"\%s\n","*Step, name=Buckle_Step, perturbation");
fprintf(fid,"\%s\n","*Buckle, eigensolver=lanczos");
fprintf(fid,"\%s\n","20, , ,");
fprintf(fid,"\%s\n","**");

%INPUT FILE GENERATION - BOUNDARY CONDITIONS
fprintf(fid,"\%s\n","** Name: Rib_Symm_BC Type: Symmetry/Antisymmetry/Encastre");
fprintf(fid,"\%s\n","*Boundary");
fprintf(fid,"\%s\n","Rib_Symm_Set, XSYMM");
fprintf(fid,"\%s\n","**");

fprintf(fid,"\%s\n","** Name: Sub_Base_BC Type: Displacement/Rotation");
fprintf(fid,"\%s\n","*Boundary");
fprintf(fid,"\%s\n","Sub_Base_Set, 1, 1");
fprintf(fid,"\%s\n","Sub_Base_Set, 2, 2");
fprintf(fid,"\%s\n","Sub_Base_Set, 3, 3");
fprintf(fid,"\%s\n","Sub_Base_Set, 4, 4");
fprintf(fid,"\%s\n","Sub_Base_Set, 5, 5");
fprintf(fid,"\%s\n","Sub_Base_Set, 6, 6");
fprintf(fid,"\%s\n","** Name: Sub_Symm_BC Type: Symmetry/Antisymmetry/Encastre");
fprintf(fid,"\%s\n","*Boundary");
fprintf(fid,"\%s\n","Sub_Symm_Set, XSYMM");

%INPUT FILE GENERATION - PRESSURE LOADS
fprintf(fid,"\%s\n","**");
fprintf(fid,"\%s\n","** LOADS");
fprintf(fid,"\%s\n","**");
fprintf(fid,"\%s\n","** NAME: FRONT_LOAD TYPE: PRESSURE");
fprintf(fid,"\%s\n","*DSLOAD");
fprintf(fid,"\%s\n","FRONT_FACE_SURF, P, 1");
fprintf(fid,"\%s\n","** NAME: BACK_LOAD TYPE: PRESSURE");
fprintf(fid,"\%s\n","*DSLOAD");
fprintf(fid,"\%s\n","BACK_FACE_SURF, P, 1");
%INPUT FILE GENERATION - OUTPUT REQUESTS
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** OUTPUT REQUESTS');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*RESTART, WRITE, FREQUENCY=0');
fprintf(fid,'%s
','*NODE PRINT, GLOBAL=YES');
fprintf(fid,'%s
',' U');
fprintf(fid,'%s
',' *NODE FILE');
fprintf(fid,'%s
',' U');
fprintf(fid,'%s
','*COORD');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*END STEP');
fprintf(fid,'%s
','**');

%DISPLAY THE ASPECT RATIO
display('')
display('')
display('The Aspect Ratio of the Film Elements is:')
display(['AXY=' num2str(alpha_xy)])
display(['AZX=' num2str(alpha_zx)])
display(['AZY=' num2str(alpha_zy)])

F.2 3-D Analysis: Post-buckling Matlab Script

% Creates Linear Brick Elements for 3D Ribbon for Post Buckling Analysis
% For an any number of layers (thickness and width) only
% Nodal Positions will work out MUCH BETTER if you use an even number of layers

clear all;
close all;
cle

% MODEL PARAMETERS
HS = 500; %Substrate thickness [micron]
L = 200; %Ribbon Length [micron]
W = 1; %Ribbon width [micron] - Actually half the width due to the symmetry bounary condition
H = 0.1; %Ribbon thickness [micron]
dze = 750; %Number of element divisions down ribbon length (Ensure this matches up with mesh of substrate)
dye = 2; %Number of element divisions through ribbon thickness (EVEN NUMBER IS ADVISED)
dxe = 6; %Number of element divisions down ribbon width (EVEN NUMBER IS ADVISED)
dzn = dze+1; %Number of node layers down ribbon length
dyn = dye+1; %Number of node layers through ribbon thickness
dxn = dxe+1; %Number of node layers down ribbon width
cye = 0; %Element layer counter (thickness)
cxe = 0; %Element layer counter (width)
cyn = 0; %Node layer counter (thickness)
cxn = 0; %Node layer counter (width)
\% FILM ELEMENT ASPECT RATIO
D_z = L/d_z;
D_y = H/d_y;
D_x = W/d_x;
alpha_{xy} = D_x/D_y;
alpha_{zx} = D_z/D_x;
alpha_{zy} = D_z/D_y;

\%OUTPUT FILE SPECIFICATION
fid = fopen('buckle_3d_out.txt','w');

\%INPUT FILE GENERATION - HEADING
fprintf(fid,'%s
','*HEADING');
fprintf(fid,'%s
',[' LINEAR BUCKLING: X,Y,Z DIV = ' num2str(d_x) ', ' num2str(d_y) ', '
 num2str(d_z) ' (' num2str(H*1000) ' nm THICK)']);
fprintf(fid,'%s
','** JOB NAME: Buckle MODEL NAME: Buckle_Model');
fprintf(fid,'%s
','** Preprint, echo=NO, model=NO, history=NO, contact=NO');
fprintf(fid,'%s
','**

\%INPUT FILE GENERATION - PART DEFINITION
fprintf(fid,'%s
','** PARTS');
fprintf(fid,'%s
','**
fprintf(fid,'%s
','*PART, NAME=BULK_3D');
fprintf(fid,'%s
','*END PART');
fprintf(fid,'%s
','**
fprintf(fid,'%s
','*PART, NAME=INT_3D');
fprintf(fid,'%s
','*END PART');
fprintf(fid,'%s
','**
fprintf(fid,'%s
','*PART, NAME=RIB_3D');
fprintf(fid,'%s
','*END PART');
fprintf(fid,'%s
','**

\%INPUT FILE GENERATION - ASSEMBLY
fprintf(fid,'%s
','** ASSEMBLY');
fprintf(fid,'%s
','**
fprintf(fid,'%s
','*ASSEMBLY, NAME=ASSEMBLY');
fprintf(fid,'%s
','**

\%INPUT FILE GENERATION - RIBBON NODES/ELEMENTS
fprintf(fid,'%s
','*INSTANCE, NAME=BULK_3D_INST, PART=BULK_3D');
fprintf(fid,'%s
','*End Instance');
fprintf(fid,'%s
','**
fprintf(fid,'%s
','*Nset, nset=_PickedSet2, internal, generate');
fprintf(fid,'%s
','     1,  44804,      1');
fprintf(fid,'%s
','*Elset, elset=_PickedSet2, internal, generate');
fprintf(fid,'%s
','      1,  202524,       1');
fprintf(fid,'%s
','** Section: Sub_Sec');
fprintf(fid,'%s
','*Solid Section, elset=_PickedSet2, material=Sub_Prop');
fprintf(fid,'%s
','1.,');
fprintf(fid,'%s
','*End Instance');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*INSTANCE, NAME=INT_3D_INST, PART=INT_3D');
fprintf(fid,'%s
','         4.5,           0.,           0.);
fprintf(fid,'%s
',' ').
fprintf(fid,'%s
',' ').
fprintf(fid,'%s
','---------- INSERT SUBSTRATE NODES & ELEMENTS HERE ----------');
fprintf(fid,'%s
','
').
fprintf(fid,'%s
','*Nset, nset=_PickedSet2, internal, generate');
fprintf(fid,'%s
','     1,  99883,      1');
fprintf(fid,'%s
','*Elset, elset=_PickedSet2, internal, generate');
fprintf(fid,'%s
','     1,  81000,      1');
fprintf(fid,'%s
','** Section: Sub_Sec');
fprintf(fid,'%s
','*Solid Section, elset=_PickedSet2, material=Sub_Prop');
 fprintf(fid,'%s
','1.,');
fprintf(fid,'%s
','*End Instance');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*INSTANCE, NAME=RIB_3D_INST, PART=RIB_3D');
fprintf(fid,'%s
',
'        0,       ' num2str(HS) ',           0');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** RIBBON NODE GENERATION');
fprintf(fid,'%s
','**');
for cyn = 1:dyn
      for cxn = 1:dxn
            fprintf(fid,'%s
','*NODE');
            fprintf(fid,'%s
',[num2str((cyn-1)*dxn*dzn+(cxn-1)*dze+cxn) ', ' num2str(W-(cxn-1)/dxe*W) ', ' num2str(H-(cyn-1)/dye*H) ',' num2str(0)]);
            fprintf(fid,'%s
',[num2str((cyn-1)*dxn*dzn+cxn*dze+cxn) ', ' num2str(W-(cxn-1)/dxe*W) ', ' num2str(H-(cyn-1)/dye*H) ',' num2str(-L)]);
      end
end
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** RIBBON ELEMENT GENERATION');
fprintf(fid,'%s
','**');
for cye = 1:dye
      for cxe = 1:dxe
            fprintf(fid,'%s
','*ELEMENT, TYPE=C3D8R');
            fprintf(fid,'%s
',[num2str((cxe-1)*dze+(cye-1)*dxn*dnz) ', ' num2str((cxe-1)*dze+cxe+(cye-1)*dxn*dnz+1) ', ' num2str((cxe-1)*dze+cxe+cye*dxn*dnz+2) ', ' num2str((cxe-1)*dze+cxe+cye*dxn*dnz+2) ', ' num2str((cxe-1)*dze+cxe+cye*dxn*dnz+1) ', ' num2str((cxe-1)*dze+cyce+cxye*dxn*dnz+1) ', ' num2str((cxe-1)*dze+cyce+cxye*dxn*dnz+1) ', ' num2str((cxe-1)*dze+cyce+cxye*dxn*dnz+1) ']);
      end
end
fprintf(fid,'%s
','
')
fprintf(fid,'%s','*ELGEN');
fprintf(fid,'%s',[num2str((cxe-1)*dze+(cye-1)*dxe*dze+1) ', ' num2str(dze) ', ' num2str(1) ',
1']);
end
end

fprintf(fid,'%s','*NSET, NSET=RIB_SET, INSTANCE=RIB_3D_INST, INTERNAL,
GENERATE');
fprintf(fid,'%s',[num2str(1) ', ' num2str(dxn*dyn*dzn) ', ' num2str(1) ]);fprintf(fid,'%s','*ELSET, ELSET=RIB_SET, INSTANCE=RIB_3D_INST, INTERNAL,
GENERATE');
fprintf(fid,'%s',[num2str(1) ', ' num2str(dxe*dye*dze) ', ' num2str(1) ]);fprintf(fid,'%s','** SECTION: REB_SEC');fprintf(fid,'%s','*SOLID SECTION, ELSET=RIB_SET, MATERIAL=RIB_PROP');fprintf(fid,'%s','1');fprintf(fid,'%s','**');fprintf(fid,'%s','*END INSTANCE');fprintf(fid,'%s','**');fprintf(fid,'%s','** SETS FOR ANALYSIS');fprintf(fid,'%s','**');fprintf(fid,'%s','** SYMMETRY SETS');fprintf(fid,'%s','**');fprintf(fid,'%s','**RIBBON');fprintf(fid,'%s','*** SECTION: REB_SEC');fprintf(fid,'%s','*SOLID SECTION, ELSET=RIB_SET, MATERIAL=RIB_PROP');fprintf(fid,'%s','');fprintf(fid,'%s','---------- INSERT SYMM SETS FOR BULK SUBSTRATE ----------');fprintf(fid,'%s','');fprintf(fid,'%s','*NSET, NSET=SUB_SYMM_SET, INSTANCE=INT_3D_INST,
');fprintf(fid,'%s','**SUBSTRATE');fprintf(fid,'%s','*NSET, NSET=SUB_SYMM_SET, INSTANCE=INT_3D_INST,
GENERATE');fprintf(fid,'%s','---------- INSERT SYMM SETS FOR INTERFACE SUBSTRATE ----------');fprintf(fid,'%s','**');fprintf(fid,'%s','*ELSET, ELSET=SUB_SYMM_SET, INSTANCE=BULK_3D_INST');fprintf(fid,'%s','');fprintf(fid,'%s','**');fprintf(fid,'%s','*ELSET, ELSET=SUB_SYMM_SET, INSTANCE=INT_3D_INST,'
fprintf(fid,'%s
','---------- INSERT SYMM SETS FOR BULK SUBSTRATE ----------');
fprintf(fid,'%s
',' *ELSET, ELSET=SUB_SYMM_SET, INSTANCE=INT_3D_INST, GENERATE');
fprintf(fid,'%s
','---------- INSERT SYMM SETS FOR INTERFACE SUBSTRATE ----------');
fprintf(fid,'%s
','---------- INSERT BASE SETS FOR INTERFACE SUBSTRATE ----------');
fprintf(fid,'%s
','---------- INSERT BASE SETS FOR BULK SUBSTRATE ----------');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** BOUNDARY CONDITION SETS');
fprintf(fid,'%s
','**SUBSTRATE');
fprintf(fid,'%s
','*NSET, NSET=SUB_BASE_SET, INSTANCE=BULK_3D_INST');
fprintf(fid,'%s
','---------- INSERT BASE SETS FOR INTERFACE SUBSTRATE ----------');
fprintf(fid,'%s
','---------- INSERT BASE SETS FOR BULK SUBSTRATE ----------');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** RIBBON NODE & ELEMENT SETS');
fprintf(fid,'%s
','**TIE CONSTRAINT SETS & SURFACES');
fprintf(fid,'%s
','** BULK-INTERFACE: BULK');
fprintf(fid,'%s
','*Elset, elset=_Bulk_Inter_Bot_Tie_Surf_S3, internal, instance=BULK_3D_INST');
fprintf(fid,'%s
','---------- INSERT TIE SETS FOR BOTTOM BULK-INTERFACE ----------');
fprintf(fid,'%s
','---------- INSERT TIE SETS FOR BOTTOM BULK-INTERFACE ----------');
fprintf(fid,'%s
','*Surface, type=ELEMENT, name=Bulk_Inter_Bot_Tie_Surf');
fprintf(fid,'%s\n','*Elset, elset=_Bulk_Inter_Bot_Tie_Surf_S3, internal, instance=BULK_3D_INST);
fprintf(fid,'%s\n','---------- INSERT TIE SETS FOR BOTTOM BULK-INTERFACE ----------');
fprintf(fid,'%s\n','*Elset, elset=_Bulk_Inter_Bot_Tie_Surf_S4, internal, instance=BULK_3D_INST);
fprintf(fid,'%s\n','---------- INSERT TIE SETS FOR BOTTOM BULK-INTERFACE ----------');
fprintf(fid,'%s\n','*Elset, elset=_Bulk_Inter_Bot_Tie_Surf_S2, internal, instance=BULK_3D_INST);
fprintf(fid,'%s\n','---------- INSERT TIE SETS FOR BOTTOM BULK-INTERFACE ----------');
fprintf(fid,'%s\n','*Elset, elset=_Bulk_Inter_Bot_Tie_Surf_S1, internal, instance=BULK_3D_INST);
fprintf(fid,'%s\n','---------- INSERT TIE SETS FOR BOTTOM BULK-INTERFACE ----------');
fprintf(fid,'%s\n','*Surface, type=ELEMENT, name=Bulk_Inter_Bot_Tie_Surf');
fprintf(fid,'%s\n','_Bulk_Inter_Bot_Tie_Surf_S3, S3');
fprintf(fid,'%s\n','_Bulk_Inter_Bot_Tie_Surf_S4, S4');
fprintf(fid,'%s\n','_Bulk_Inter_Bot_Tie_Surf_S2, S2');
fprintf(fid,'%s\n','_Bulk_Inter_Bot_Tie_Surf_S1, S1');
fprintf(fid,'%s\n','**');

fprintf(fid,'%s\n','** BULK-INTERFACE: INTERFACE');
fprintf(fid,'%s\n','*Elset, elset=_Inter_Bulk_Bot_Tie_Surf_S5, internal, instance=INT_3D_INST);
fprintf(fid,'%s\n','---------- INSERT TIE SETS FOR BOTTOM BULK-INTERFACE ----------');
fprintf(fid,'%s\n','*Surface, type=ELEMENT, name=Inter_Bulk_Bot_Tie_Surf');
fprintf(fid,'%s\n','_Inter_Bulk_Bot_Tie_Surf_S5, S5');
fprintf(fid,'%s\n','*Elset, elset=_Inter_Bulk_Bot_Tie_Surf_S4, internal, instance=INT_3D_INST, generate); 
fprintf(fid,'%s\n','---------- INSERT TIE SETS FOR BULK-INTERFACE ----------');
fprintf(fid,'%s\n','---------- INSERT TIE SETS FOR RIBBON-INTERFACE ----------');
fprintf(fid,'%s\n','*Surface, type=ELEMENT, name=Inter_Bulk_Bot_Tie_Surf');
fprintf(fid,'%s\n','_Inter_Bulk_Bot_Tie_Surf_S4, S4');
fprintf(fid,'%s\n','**');

fprintf(fid,'%s\n','** INTERFACE-RIBBON: INTERFACE');
fprintf(fid,'%s\n','*Elset, elset=_Inter_Rib_Tie_Surf_S3, internal, instance=INT_3D_INST);
fprintf(fid,'%s\n','---------- INSERT TIE SETS FOR RIBBON-INTERFACE ----------');
fprintf(fid,'%s\n','---------- INSERT TIE SETS FOR RIBBON-INTERFACE ----------');
fprintf(fid,'%s\n','---------- INSERT TIE SETS FOR RIBBON-INTERFACE ----------');
fprintf(fid,'%s\n','---------- INSERT TIE SETS FOR RIBBON-INTERFACE ----------');
fprintf(fid, '%s
', '_Inter_Rib_Tie_Surf_S3, S3');
fprintf(fid, '%s
', '*ELSET, ELSET=RIB_INT_TIE_SET, INSTANCE=RIB_3D_INST, GENERATE');
fprintf(fid, '%s
', num2str((dye-1)*dxe*dze+1), ', ', num2str(dye*dxe*dze), ', ', num2str(1));
fprintf(fid, '%s
', 'RIB_INT_TIE_SET, S5');
fprintf(fid, '%s
', '*INTERFACE-RIBBON: RIBBON');
fprintf(fid, '%s
', '*SURFACE, TYPE=ELEMENT, NAME=Rib_Inter_Tie_Surf');
fprintf(fid, '%s
', '*Tie, name=Inter_Bulk_Bot_TC, adjust=yes');
fprintf(fid, '%s
', 'Bulk_Inter_Bot_Tie_Surf, Inter_Bulk_Bot_Tie_Surf');
fprintf(fid, '%s
', '*Tie, name=Inter_Bulk_Side_TC, adjust=yes');
fprintf(fid, '%s
', 'Bulk_Inter_Side_Tie_Surf, Inter_Bulk_Side_Tie_Surf');
fprintf(fid, '%s
', '*Tie, name=Rib_Inter_TC, adjust=yes');
fprintf(fid, '%s
', 'Inter_Rib_Tie_Surf, Rib_Inter_Tie_Surf');
fprintf(fid, '%s
', '*Material, name=Rib_Prop');
fprintf(fid, '%s
', '*Elastic');
fprintf(fid, '%s
', '130000., 0.3');
fprintf(fid, '%s
', '*Expansion');
fprintf(fid, '%s
', '2.6e-06,');
fprintf(fid, '%s
', '*Material, name=Sub_Prop');
fprintf(fid, '%s
', '*Elastic');
fprintf(fid, '%s
', '2., 0.49');
fprintf(fid, '%s
', '*Expansion');
fprintf(fid, '%s
', '0.00034,');
fprintf(fid, '%s
', '----------------------------------------------------------------');
fprintf(fid, '%s
', '----------------------------------------------------------------');
%INPUT FILE GENERATION - BOUNDARY CONDITIONS
fprintf(fid,'%s','** Name: Rib_Symm_BC Type: Symmetry / Antisymmetry / Encastre');
fprintf(fid,'%s','*Boundary');
fprintf(fid,'%s','Rib_Symm_Set, XSYMM');
fprintf(fid,'%s');
fprintf(fid,'%s','** Name: Sub_Base_BC Type: Displacement/Rotation');
fprintf(fid,'%s','*Boundary');
fprintf(fid,'%s','Sub_Base_Set, 1, 1');
fprintf(fid,'%s','Sub_Base_Set, 2, 2');
fprintf(fid,'%s','Sub_Base_Set, 3, 3');
fprintf(fid,'%s','Sub_Base_Set, 4, 4');
fprintf(fid,'%s','Sub_Base_Set, 5, 5');
fprintf(fid,'%s','Sub_Base_Set, 6, 6');
fprintf(fid,'%s','** Name: Sub_Symm_BC Type: Symmetry / Antisymmetry / Encastre');
fprintf(fid,'%s');
fprintf(fid,'%s','**');
fprintf(fid,'%s','**');
fprintf(fid,'%s','**');
fprintf(fid,'%s','**');
%INPUT FILE GENERATION - LOAD STEP (LINEAR/STATIC)
fprintf(fid,'%s','** STEP: Step-1');
fprintf(fid,'%s','*STEP, NLGEOM=YES');
fprintf(fid,'%s','*STATIC');
fprintf(fid,'%s','0.01, 15, 0.0001, 0.1');
fprintf(fid,'%s');
%INPUT FILE GENERATION - TEMPERATURE FIELD
fprintf(fid,'%s','** PREDEFINED FIELDS');
fprintf(fid,'%s','**');
fprintf(fid,'%s','** Name: Temp_Field Type: Temperature');
fprintf(fid,'%s','*Temperature');
fprintf(fid,'%s','Rib_Set, 57692.');
%INPUT FILE GENERATION - OUTPUT REQUESTS
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** OUTPUT REQUESTS');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*RESTART, WRITE, FREQUENCY=1');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** FIELD OUTPUT: OUT_REQUEST');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*OUTPUT, FIELD');
fprintf(fid,'%s
','*NODE OUTPUT');
fprintf(fid,'%s
',' NT, U');
fprintf(fid,'%s
','*ELEMENT OUTPUT, DIRECTIONS=YES');
fprintf(fid,'%s
',' TEMP, S, E, LE, EP, THE');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** HISTORY OUTPUT: OUT_REQUEST');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*OUTPUT, HISTORY');
fprintf(fid,'%s
','*ENERGY OUTPUT');
fprintf(fid,'%s
','ETOTAL, ALLSE, ALLSD, ALLIE, ALLAE');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** PRINT RESULTS');
fprintf(fid,'%s
','*EL PRINT, ELSET=RIB_SET, FREQUENCY=10');
fprintf(fid,'%s
',' S');
fprintf(fid,'%s
',' E');
fprintf(fid,'%s
',' THE');
fprintf(fid,'%s
','*EL FILE, FREQUENCY=10');
fprintf(fid,'%s
',' S');
fprintf(fid,'%s
',' E');
fprintf(fid,'%s
',' THE');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','** PRINT NODAL RESULTS');
fprintf(fid,'%s
','*NODE PRINT, NSET=RIB_SET, FREQUENCY=10');
fprintf(fid,'%s
',' U, NT');
fprintf(fid,'%s
','*NODE FILE, FREQUENCY=10');
fprintf(fid,'%s
',' U, NT');
fprintf(fid,'%s
','**');
fprintf(fid,'%s
','*END STEP');
fprintf(fid,'%s
','**');

%DISPLAY THE ASPECT RATIO
display(' '); 
display(' '); 
display('The Aspect Ratio of the Film Elements is:');
display(['AXY=' num2str(alpha_xy)]);
display(['AZX=' num2str(alpha_zx)]);
display(['AZY=' num2str(alpha_zy)]);
Solving plasticity problems using finite element analysis is rooted in the incremental nature of the strain decomposition

\[ \text{d} \varepsilon = \text{d} \varepsilon^e + \text{d} \varepsilon^p \]  \hspace{1cm} (G.1)

Abaqus uses associated flow theory (meaning the flow of plastic strain is associated with the yield condition directly) according to von Mises failure criterion for metallic plasticity according to the following

\[ \text{d} \varepsilon^p = \text{d} \lambda \frac{\partial F}{\partial \sigma} \]  \hspace{1cm} (G.2)

\[ F = J_2 - k^2 = 0 \]  \hspace{1cm} (G.3)

where \( \text{d} \lambda \) is the increment of a scalar constant and \( F \) is the yield surface calculated according to von Mises criterion. Note that the gradient of the yield surface to the stress is orthogonal to the yield surface (Figure G.1). The yield condition of equation (G.3) involves a parameter, \( k \), which is a specified yield stress for a given plastic strain. As stated in the main text, the material response beyond the elastic limit (initial yield surface) at the \( n+1 \) step is calculated according to linear elastic behavior (Figure G.2) as a trial quantity (denoted with an apostrophe).

\[ \Delta \sigma'_{n+1} = D \Delta \varepsilon_{n+1} \]  \hspace{1cm} (G.4)

Figure G.1 Diagram of the material response during (a) elastic deformation, (b) initial yielding, and (c) subsequent yielding.
The yield condition of equation (G.3) is then checked for the current trial state at n+1 for the plastic strain at the n increment. This is because it is assumed that no plastic straining occurs between steps n and n+1. The stress increment between the two steps is calculated according to

$$\Delta \sigma_{n+1} = D(\Delta \varepsilon_{n+1}^{\text{tot}} - \Delta \varepsilon_{n+1}^{\text{pl}})$$

where $a$ is the gradient of the yield surface to the stress state, $\frac{\partial F}{\partial \sigma}$ according to the associated flow rule. The consistency for the yield condition is then linearized around the trial state in order to determine the value for $\Delta \lambda$ according to
where $A_n$ is calculated at the previous step to be

$$A_n = \left( \frac{\partial F}{\partial \sigma} \right)^T a_n \quad (G.7)$$

Once the scalar constant is known, plastic strain at the first trial state can be calculated

$$\varepsilon_{n+1}^{pl} = \varepsilon_n^{pl} + \Delta \lambda a_n^{\prime} \quad (G.8)$$

and a new trial stress (Figure G.3) state can be calculated as well

$$\sigma_{n+1}^{\prime} = \sigma_n^{\prime} - \Delta \lambda D a_n^{\prime} \quad (G.9)$$

The yield condition at the calculated plastic strain is then checked at this new trial state. If the yield condition is violated, then iterations continue until the condition is satisfied (Figure G.4). Once the yield condition is satisfied the last trial state becomes the final state for the $n+1$ increment. The procedure continues according to this methodology for subsequent yield at $n+2$, $n+3$, $n+4$, etc. steps.
Figure G.3 Diagram of the next trial state, $\sigma''$.  

Figure G.4 Diagram showing a final converged stress state after several iterations where the last trial state becomes the final stress state for the $n+1$ step.
APPENDIX H

PLASTIC ANALYSIS MOVIES (MS WINDOWS)
The movies (placed in a single ZIP file) that accompany this thesis demonstrate the evolution of the morphology, the stress, and the plastic strain in the Si thin film.