Adsorption of silicon atom on chlorinated Si(100) surface

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Homoepitaxial growth of Si on Si(100) covered by a resist mask is a necessary technological step for the fabrication of donor-based quantum devices with STM lithography. Using density functional theory, we investigated the adsorption of a single silicon atom on Si(100)-2×1-Cl as the starting process of Si epitaxy. The incorporation of a silicon atom under Cl monolayer proved to be the most energetically favorable process. In the course of spontaneous adsorption, one Si adatom substitutes one Cl atom. Then, the adatom can migrate to more stable adsorption sites forming bonds with two Si and two Cl atoms, but this process requires activation energy. In addition, we found that at Si adsorption, SiCl\textsubscript{2}, SiCl\textsubscript{3}, and SiCl\textsubscript{4} clusters can be formed above a Si(100)-2×1-Cl surface. SiCl\textsubscript{2} clusters are bound weakly to the substrate, and their desorption leaves the silicon surface free of chlorine. Our results show that chlorine segregates to the surface during Si deposition and does not incorporate into homoepitaxial layers.

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I. INTRODUCTION

Homoepitaxy of silicon is widely utilized for dopant encapsulation in atomic scale devices. Sufficiently thick crystalline silicon layer (about 50 nm) should be grown on top of a surface with dopants to preserve the electronic properties of semiconducting devices from unwanted surface effects. Silicon epitaxy is a necessary step for the fabrication of δ-layers\textsuperscript{12}, nanowires\textsuperscript{3,4}, and quantum dots\textsuperscript{5}. In addition, a high quality of epitaxial layers is extremely important for phosphorus-in-silicon quantum computer building blocks\textsuperscript{6,7}.

To create the desired two-dimensional structure of impurities, a silicon surface is covered with a resist and then the resist is patterned with a scanning tunneling microscope (STM) tip. After the adsorption of molecules containing specific impurities, the impurity atoms are embedded on the resist-free sites and then the surface is covered with epitaxial silicon layers. The quality of epitaxial layers strongly depends on the interaction of Si adatoms with atoms of the resist used for mask fabrication. If a hydrogen monolayer is used as a mask for the patterning of Si(100)-2×1 surface, the uniform growth of an epitaxial Si film is suppressed at room temperature\textsuperscript{8,9} due to low mobility of Si adatoms\textsuperscript{10}. The surface roughness of the film can be decreased by sample heating, as in the case of Si epitaxy on clean Si(100)\textsuperscript{11,16}. However, to prevent the lateral diffusion of dopants, heating to temperatures at which hydrogen begins to desorb (above 400°C\textsuperscript{12}) should be avoided.

Theoretical calculations of Si atoms adsorption and diffusion on H-terminated Si(100)-2×1 surface have provided insight into mechanism of homoepitaxy\textsuperscript{10,13,14}. A silicon atom adsorbed on Si(100)-2×1-H can spontaneously substitute a hydrogen atom on the surface and then form Si dihydride. Experimental results confirm the presence of surface Si dihydrides at sub-monolayer coverages\textsuperscript{15}. As such a Si film grows, most H atoms segregate to the surface and are not incorporated into the epitaxial film\textsuperscript{11,16}.

Chlorine monolayer on a silicon surface can also be utilized as a resist\textsuperscript{17,18}. Of particular interest is a proposal to use STM lithography on Si(100)-2×1-Cl for placing P atoms with atomic precision\textsuperscript{19}. However, the atomic processes of silicon epitaxy on a Cl-terminated Si(100)-2×1 surface have not been studied either theoretically or experimentally.

In this paper, we report the results of density functional theory (DFT) calculations of Si atom adsorption on Si(100)-2×1-Cl. A silicon adatom spontaneously substitutes a Cl atom and further migrates to the most stable inter-bridge dimer site (bound with two Si and two Cl atoms). This process is similar to that in the case of Si(100)-2×1-H surface, and should lead to Cl atoms segregation during Si epitaxy. Despite the small radius of hydrogen being suggested\textsuperscript{11} as a reason for spontaneous substitutional adsorption of silicon on Si(100)-2×1-H, the same adsorption mechanism is found to work for a chlorinated silicon surface. Moreover, there is an additional pathway of spontaneous Si adsorption with formation of SiCl\textsubscript{2} clusters weakly bound with the silicon surface. The spontaneous desorption of SiCl\textsubscript{2} clusters from the surface makes it possible to remove chlorine without annealing.

II. CALCULATION METHOD

First-principle calculations of silicon atom adsorption on Si(100)-2×1-Cl surface were performed with spin-polarized density functional theory implemented in VASP\textsuperscript{20,21}. The generalized gradient approximation with the exchange-correlation functional in the form of Perdew–Burke–Ernzerhof (PBE) was applied\textsuperscript{22}. The eigenfunctions of valence electrons were expanded in a plane waves basis set with an energy cutoff of 350 eV. The Si(100) surface was simulated by recurring 4×4 cells.
consisted of eight atomic layers of silicon. The slabs were separated by vacuum gaps of approximately 15 Å. The bottom three layers were fixed at bulk positions, while the other silicon layers were allowed to relax. The lowest layer was covered by hydrogen atoms to saturate the broken bonds of silicon. Chlorine atoms were placed on the upper side of the slab to form a Si(100)-2×1-Cl structure. Reciprocal cell integrations were performed using the 4×4×1 k-points grid.

The adsorption energy \( E_{ads} \) of a silicon adatom was calculated as the difference between the total energy of the slab with the adatom \( (E_{Si+surf}) \) and the total energies of the Si(100)-2×1-Cl surface \( (E_{surf}) \) and a Si atom in the gaseous phase \( (E_{Si}) \):

\[
E_{ads} = E_{Si+surf} - E_{surf} - E_{Si}.
\]

The activation barriers \( E_{act} \) were calculated using the NEB (nudged elastic band) method\(^\text{23} \) implemented in VASP.

### III. RESULTS

To investigate a potential energy surface for Si adsorption on Si(100)-2×1-Cl, Si adatom \( (\text{Si}_{\text{ad}}) \) was placed 2.50 Å above the chlorine monolayer (Fig. 1a). Eight different initial configurations \( (A_0–H_0) \) of the silicon adatom above the Si(100)-2×1-Cl surface were tested (Fig. 1b). Structures A–H obtained after the optimization of the corresponding initial configurations \( A_0–H_0 \) are shown in Fig. 2.

![Figure 1](image1.png)

**Figure 1.** Perspective (a) and top (b) views of initial configurations of Si(100)-2×1-Cl with Si adatom above the surface. Silicon bulk and surface atoms are small and big yellow circles, respectively; chlorine atoms are green circles; Si adatom is orange circle.

![Figure 2](image2.png)

**Figure 2.** Optimized atomic structures and their adsorption energies for Si adsorbed on Si(100)-2×1-Cl. Structures A–H were obtained as a result of the relaxation of the coordinates when the Si adatom was in the initial positions \( A_0–H_0 \) (Fig. 1b), whereas for structures J and K adatom was initially placed close to the final positions.

In symmetric positions \( A_0 \) and \( B_0 \) (Fig. 1b), the adatom forms two equivalent bonds with Cl atoms belonging to different dimers (structures A and B in Fig. 2). Both optimized models (A and B) have the same Si–Cl bond lengths (2.09 Å) and the Cl–Si\(_{\text{ad}}\)–Cl angle of 102°. These structural parameters appear to be equal to those calculated for the SiCl\(_2\) molecule in vacuum (2.09 Å and 102°). Note also that the formation of the SiCl\(_2\) clusters is accompanied by the lengthening of the distances between Cl and Si surface atoms. In particular, the Cl–Si distances for models A and B are 4.28 Å and 3.26 Å, respectively, which is longer than the Si–Cl bond length
of an unperturbed Si(100)-2×1-Cl surface (2.08 Å). This effect indicates a rather weak interaction of the SiCl,
cluster with the surface. However, the adsorption energies of the Si adatom remain negative for models A and
B (−1.14 eV and −0.88 eV, respectively).

Two other SiCl,
clusters were obtained from the Si,
initial adsorption position on top of a Cl atom (C0 in
Fig. 1b) and from a position shifted by 0.50 Å across the
dimer row (D0 in Fig. 1b). However, the geometry of
SiCl,
clusters in models C and D (Fig. 2) differs from
that of a SiCl,
molecule. Indeed, in model C (model
D), the distance between the Si,
and the upper chlorine atom is 2.06 Å (2.03 Å), whereas the distance between the
Si,
and the lower chlorine atom appears to be higher — 2.18 Å (2.25 Å). The angle Cl–Si–Cl (104°) is close
to that in the SiCl,
molecule (102°). Models C and D have one of the bonds between the SiCl,
cluster and the substrate silicon atom shorter than those in models A and B, respectively: the corresponding Cl–Si distances for models C and D are 2.57 Å and 2.41 Å, being much shorter than in models A (4.28 Å) and B (3.26 Å). Additionally, in model C (model
D), the bond length between the upper chlorine atom of the SiCl,
cluster and the silicon atom of the surface is increased to 3.89 Å (3.54 Å) compared with the Si–Cl bond length (2.08 Å) before the Si
adsorption.

The other stable cluster, SiCl,
, was obtained by optimiz-
ing initial configurations E0 and F0 in Fig. 1b). In
model F (Fig. 2), the SiCl,
cluster forms as a Cl atom is taken from the nearest dimer (not shown in Fig. 2) and added to the cluster. The shortest bond in such a SiCl,
cluster is between the Si,
and the upper Cl (2.08 Å), whereas the lengths of the other two Si–Cl bonds are 2.49 Å. The distance between the lower Cl atoms of the
SiCl,
cluster and Si surface atoms is 2.21 Å. Note that the SiCl,
cluster located on a bridge dimer site (model E in
Fig. 2) is energetically more favorable (−1.76 eV) than that in the inter-bridge dimer site (−1.62 eV, model F in
Fig. 2).

The optimization of the initial configuration G0 in
Fig. 1b) leads to the formation of the SiCl,
cluster (see model G in Fig. 2). In this case, all Si–Cl bonds are equivalent and characterized by the length of 2.70 Å. Ad-
sorption energy in the model G (−1.44 eV) appears to be compatible with Eads calculated for configurations contain-
ing SiCl2 and SiCl3 clusters (see Fig. 2).

Optimizing initial configuration H0 (Fig. 1b), we get a Si
adatom embedding in the silicon lattice, and the chlor-
ine segregated on top of the surface structure (model H in
Fig. 2). The bond length between the Si adatom and the nearest Si atom is a little longer than in the bulk (2.50 Å vs 2.37 Å). The bond between the adatom and the second-layer substrate atom is also longer, 3.80 Å. The Si–Cl bond length (2.09 Å) appears to be close to the reference Si–Cl values of the bond length of an unperturbed Si(100)-2×1-Cl surface. Therefore, all structures formed during spontaneous adsorption of a si-
licon atom from positions indicated in Fig. 1, substi-
tional adsorption leads to the most energetically favor-
able structure H (Eads = −2.92 eV).

Since such substitutional adsorption turned out to be
very stable, we have considered additional adsorption po-
sitions of a silicon atom under the chlorine monolayer,
that could be reached by Si migration from position
H. In the most favorable configurations, Si forms SiCl,
clusters in the inter-bridge and bridge dimer sites (mod-
els J and K in Fig. 2). In these models, the Si bind with Si surface atoms, unlike models A–G, in which it
bonds with Cl atoms only. The Si–Cl bond lengths are 2.44 Å and 2.36 Å in inter-bridge and bridge sites, respec-
tively, while the Si–Cl bond lengths are 2.05 Å for both sites. The adsorption energies calculated for models J
and K are −3.48 eV and −3.27 eV, respectively. This re-
result strongly suggests that the formation of the Si–Cl bonds makes a valuable contribution to the lowing of the adsorption energy in comparison with the formation of Si–Cl bonds only. Thus, atomic configuration J appears to be the most stable structure of all considered in this paper.

Figure 3 shows the energy diagram describing the pro-
cesses of SiCl,
adsorption on Si(100)-2×1-Cl and desorption
of SiCl2, SiCl3, and SiCl4 clusters. The lower part of
the diagram corresponds to the formation of bonds
between the Si adatom and Si and Cl atoms (Cl–Si–Si),
while the upper part shows the formation of bonds
between the adatom and Cl atoms only (Si–Cl–Cl).

All the structures in the upper part of the diagram
(Fig. 3) can be formed as a result of spontaneous adsorp-
tion. For each cluster, we have tested possible desorption paths. In models A and C, a SiCl,
cluster desorbs over a rather low activation barrier (Eact < 0.1 eV), while in models B and D, it desorbs spontaneously, without any barrier. Therefore, as soon as a SiCl,
cluster forms on the surface, it can desorb as a SiCl3
molecule. The SiCl3 cluster desorbs from configuration F over the activation barrier equal to the energy difference between the initial and final states. However, this difference is bigger (1.57 eV) than that of the SiCl4 desorption. A
SiCl4 cluster can desorb from model G, but it requires the highest activation barrier of 3.09 eV.

Formation of bonds between the adatom and Si surface
atoms stabilizes the structure, putting models H, J, and
K in the lower part of the diagram (Fig. 3). Configuration
H may be the result of the spontaneous relaxation of initial model H0 (Fig. 1), but also of a transition from configuration B without any activation barrier. Further,
the Si adatom adsorbed in the substitutional site can
attach a chlorine atom from the nearest dimer and mi-
grate to the most stable inter-bridge dimer site (model
J). However, this pathway requires the activation energy
of 0.71 eV. The alternative process is the adatom transi-
tion to the SiCl2 cluster in the bridge dimer site (model
K). This process would not be the energetically preferred
one, since model K is less favorable by 0.21 eV and the activation barrier for an H→K transition is higher by
0.08 eV than that for an H→J transition.
position from the substitutional site to SiH
spectrally, and the activation barriers for Si adatom trans-
gration structure by 0.5 eV and 0.6 eV, re-
gery of these structures are lower than that of the sub-
cluster or an inter-bridge dimer site. The adsorption en-
structures J and K is highly suppressed compared with
H-terminated one. In the latter case, the Si adatom,
sorption on a Cl-terminated Si(100)-2\times 1 surface with
energy (0.5 eV). Further diffusion of the SiH\textsubscript{2} cluster into the
requires an activation energy of 1.1 eV, which can be hardly
room temperature. This scenario is in agree-
stable configurations with a SiCl\textsubscript{2} cluster (mod-
els J and K in Fig. 2). According to our calculations,
minimum energy path from model H to model K re-
energy barriers appear to be very low (\textlesssim 0.1 eV) or even
non-existent. The desorption of the SiCl\textsubscript{2} species leads
to the partial removal of chlorine from a Si(100)-2\times 1-Cl surface,
and the subsequent Si overgrowth on the sub-
strate area free of Cl should increase the adatom mo-
ility (for example, the Si adatom mobility on Si(100)-
1 surfaces terminated by hydrogen (0.5–0.6 eV
is lower than that on a clean surface). This in turn leads
to a more uniform growth of the epitaxial layer. The low
temperature removal of Cl will not lead to the diffusion
of dopants (for example, P atoms) on the surface.
Therefore, when compared to the common practice of
using a hydrogen monolayer as a resist, a chlorine mono-
layer presents not just analogies, but also potential ad-
antages because of low temperature removal of chlorine
during Si epitaxy. Firstly, spontaneous substitutional
adsorption takes place both on H\textsubscript{15} and Cl-terminated
Si(100)-2\times 1. Secondly, the most stable sites for Si\textsubscript{ad} on
H\textsubscript{15} (or Cl-) terminated surfaces are bridge and inter-
bridge dimer sites, where the Si\textsubscript{ad} is bound to two Si and
two H (or Cl) atoms. Thirdly, the energy barriers for Si transition from the substitutional adsorption site to
these stable sites are similar for hydrogen (0.5–0.6 eV\textsubscript{15})
and chlorine (0.7–0.8 eV) monolayers. Fourthly, we have
found out that SiCl\textsubscript{2} clusters formed during silicon ad-
sorption can easily desorb from a Cl-terminated surface.
Thus, depositing silicon on a chlorine monolayer should
produce silicon epitaxial layers of quality at least not

\textbf{IV. DISCUSSION}

In this section, we turn to the comparison of Si ad-
sorption on a Cl-terminated Si(100)-2\times 1 surface with
a H-terminated one. In the latter case, the Si adatom,
spontaneously substituting a hydrogen atom\textsuperscript{15}, can cap-
ture one more H atom and form a SiH\textsubscript{2} cluster in a bridge
dimer or an inter-bridge dimer site. The adsorption en-
geries of these structures are lower than that of the sub-
stitutional adsorption structure by 0.5 eV and 0.6 eV, re-
spectively, and the activation barriers for Si adatom trans-
transition from the substitutional site to SiH\textsubscript{2} cluster in the
bridge dimer or inter-bridge dimer site are 0.5 eV and
0.6 eV, respectively\textsuperscript{15}. At room temperature, most of the
adsorbed Si atoms transfer from the substitutional site to the bridge dimer site due to the low activation energy
(0.5 eV). Further diffusion of the SiH\textsubscript{2} cluster into the
most favorable position in the inter-bridge dimer site
requires an activation energy of 1.1 eV, which can be hardly
overcome at room temperature. This scenario is in agree-
ment with the experiment\textsuperscript{15}, where Si atoms deposited
on a H-terminated Si(100)-2\times 1 surface at room tempera-
ture were found predominantly in the bridge dimer sites.

Like in the previous case, a silicon atom adsorbed on a
Si(100)-2\times 1-Cl surface spontaneously substitutes a chlo-
rine atom (model H in Fig. 2). Then the Si adatom can
capture an additional chlorine atom, thus creating the
more stable configurations with a SiCl\textsubscript{2} cluster (mod-
els J and K in Fig. 2). According to our calculations,
minimum energy path from model H to model K re-
quires an activation energy of 0.79 eV, whereas the trans-
ition from model H to the most stable structure (model
J) requires only 0.71 eV. Thus, our results indicate that
most Si adatoms deposited on a Si(100)-2\times 1-Cl surface
at room temperature are adsorbed into the inter-bridge
dimer site, while on a Si(100)-2\times 1-H surface Si adatoms
occupy mostly the bridge dimer sites.

Another difference between Si adsorption on Si(100)-
2\times 1-Cl and Si(100)-2\times 1-H is that in the formed case,
SiCl\textsubscript{2} clusters weakly bound to the Cl-terminated sur-
face are formed. A SiCl\textsubscript{2} molecule can easily desorb from
structures A–D containing SiCl\textsubscript{2} clusters, since the
energy barriers appear to be very low (\textlesssim 0.1 eV) or even
non-existent. The desorption of the SiCl\textsubscript{2} species leads
to the partial removal of chlorine from a Si(100)-2\times 1-Cl surface,
and the following Si overgrowth on the substrate area
of Cl should increase the adatom mobility (for example, the Si adatom mobility on Si(100)-
1 surfaces terminated by hydrogen (0.5–0.6 eV
is lower than that on a clean surface). This in turn leads
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found out that SiCl\textsubscript{2} clusters formed during silicon ad-
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Thus, depositing silicon on a chlorine monolayer should
produce silicon epitaxial layers of quality at least not

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{SI.png}
\caption{Potential energy diagram for Si adsorption on Si(100)-2\times 1-Cl and SiCl\textsubscript{2}, SiCl\textsubscript{3}, and SiCl\textsubscript{4} desorption. Reaction pathways with Cl-Si\textsubscript{ad}-Si bond formation are shown by red lines, adsorption and desorption pathways with Si\textsubscript{ad}-Cl bonds by blue lines. Activation barriers are indicated by arrows (energy barriers less than 0.05 eV are not shown in the diagram).}
\end{figure}
worse (may be even better) than on a hydrogen monolayer.

V. CONCLUSIONS

The structures and energetics of Si adsorption on Si(100)-2×1-Cl have been studied with the density function theory. The activation barriers for transitions between the most stable states and desorption of different SiClₓ compounds from the surface have been calculated. A Si adatom adsorbed on a Si(100)-2×1-Cl surface spontaneously substitutes a Cl atom (more preferable) or forms SiCl₂, SiCl₃, and SiCl₄ clusters. Note that the SiCl₂ clusters are bound weakly to the surface and therefore can easily desorb. A Si adatom located in the substitutional site can migrate to the most stable inter-bridge dimer site with the activation energy of 0.71 eV. Thus, our results indicate that chlorine segregates to the surface during Si deposition and is not incorporated into the epitaxial layers. Moreover, Si deposition on a Cl-terminated surface has a potential advantage compared to a H-terminated surface, since it may improve the quality of low temperature silicon epitaxy.

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1. T.-C. Shen, J.-Y. Ji, M. A. Zudov, R.-R. Du, J. S. Kline, and J. R. Tucker, Appl. Phys. Lett. 80, 1580 (2002)
2. J. Keizer, S. Koelling, P. Koenraad, and M. Simmons, ACS Nano 9, 2537 (2015).
3. B. Weber, S. Mahapatra, H. Ryu, S. Lee, A. Fuhrer, T. Reusch, D. L. Thompson, W. C. T. Lee, G. Klimeck, L. C. L. Hollenberg, and M. Simmons, Science 335, 64 (2012).
4. B. Weber, H. Ryu, Y.-H. M. Tan, G. Klimeck, and M. Y. Simmons, Phys. Rev. Lett. 113, 246802 (2014).
5. M. Fuechsle, J. Miwa, S. Mahapatra, H. Ryu, S. Lee, O. Warschkow, L. C. L. Hollenberg, G. Klimeck, and M. Simmons, Nat. Nanotechnol. 7, 242 (2012).
6. L. Oberbeck, N. J. Curson, M. Y. Simmons, R. Brenner, A. R. Hamilton, S. R. Schofield, and R. G. Clark, Appl. Phys. Lett. 81, 3197 (2002).
7. M. A. Broome, S. Gorman, M. House, S. Hile, J. Keizer, D. Keith, C. D. Hill, T. Watson, W. Baker, L. C. L. Hollenberg, and M. Simmons, Nature Communications 9 (2018).
8. D. P. Adams, S. M. Yalisove, and D. J. Eaglesham, Appl. Phys. Lett. 63, 3571 (1993).
9. L. Oberbeck, T. Hallam, N. J. Curson, M. Y. Simmons, and R. G. Clark, Appl. Surf. Sci. 212–213, 319 (2003).
10. J. Nara, T. Sasaki, and T. Ohno, Phys. Rev. Lett. 79, 4421 (1997).
11. X. Deng, P. Nambodiri, K. Li, X. Wang, G. Stan, A. F. Myers, X. Cheng, T. Li, and R. M. Silver, Appl. Surf. Sci. 378, 301 (2016).
12. M. L. Yu, D. J. Vitkavage, and B. S. Meyerson, J. Appl. Phys. 59, 4032 (1986).
13. S. Jeong and A. Oshiyama, Phys. Rev. Lett. 79, 4425 (1997).
14. S. Jeong and A. Oshiyama, Phys. Rev. B 58, 12958 (1998).
15. H. Kajiyama, Y. Suwa, S. Heike, M. Fujimori, J. Nara, T. Ohno, S. Matsura, T. Hitosugi, and T. Hashizume, J. Phys. Soc. Jpn. 74, 389 (2005).
16. J.-Y. Ji and T.-C. Shen, Phys. Rev. B 70, 115309 (2004).
17. S. Moon, C. Jeon, H. Hwang, C. Hong, H. Song, H. Shin, S. Chung, and C. Park, Adv. Mater. 19, 1321 (2007).
18. C. Jeon, H.-N. Hwang, H.-J. Shin, C.-Y. Park, and C.-H. Hwang, Appl. Surf. Sci. 257, 8794 (2011).
19. T. V. Pavlova, G. M. Zhidomirov, and K. N. Eltsov, J. Phys. Chem. C 122, 1741 (2018).
20. G. Kresse and J. Hafner, Phys. Rev. B 47, 558 (1993).
21. G. Kresse and J. Furthmüller, Phys. Rev. B 54, 11169 (1996).
22. J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996).
23. H. Jónsson, G. Mills, and K. W. Jacobsen, “Nudged elastic band method for finding minimum energy paths of transitions,” in Classical and Quantum Dynamics in Condensed Phase Simulations, edited by B. J. Berne, G. Ciccotti, and D. F. Coker (1998) pp. 385–404.
24. G. J. Xu and J. H. Weaver, Phys. Rev. B 70, 165321 (2004).