



# Nanoscale simulation of the lithium ion interaction with defective silicene



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## ABSTRACT

Lithium ion drift through the porous membranes in an electric field using molecular dynamics is investigated. Mono-, bi-, tri-, and hexa-vacancies were pores of two-layer silicene. Ion has a convoluted path. The average time for an ion to overcome membranes with single vacancies is more than three times higher than that for membranes with hexa-vacancies. Passage of the lithium ion through a flat silicene channel causes an increase in the roughness of the silicene, an increase in the mobility of Si atoms, a significant increase in the  $\sigma_{zx}$  stress component due to the electrostatic force action.

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## 1. Introduction

Silicene, the silicon analogue of graphene, has a large theoretical capacity and low migration energy barriers [1,2]. Therefore it is an excellent 2D anode material for lithium-ion batteries. However, the currently obtained silicene cannot be separated from the substrate. In addition as a rule silicene is deposited on metal substrates like Ag(111) and Ir(111) [3,4]. As a consequence it may lose its attractive properties such as a massless Dirac fermion character to charge carriers. Silicene can no longer be regarded as a promising anode material if it needs to be used with its substrate [5]. Theoretical studies indicate a strong bond of silicene to the substrate [6]. The use of silicene as an anode material implies its separation from the substrate. This operation will inevitably lead to the appearance of different types of defects in silicene. In this connection it is important to know how the mechanical stability of defective silicene will change and how the presence of a defect will affect the interaction of silicene with the lithium ion. These issues have not yet been considered. This problem can be solved by the method of classical molecular dynamics, which, unlike ab initio calculations, makes it possible to trace the motion of lithium ion through a two-layer silicene both horizontally and vertically over a significant time interval. The surface area and porosity of the material are two important physical quantities, which significantly

affect the efficiency of future devices. It can be expected that in two layer silicene the structural defects like poly-vacancies possibly create additional ways of passage of lithium through planes and its mobility will be increased. Intercalation of lithium ion into a two-layer silicene usually causes deformation, the extent of which does not exceed 3–4 nm. A deformation extends to the same distance when the lithium ion gets stuck between the silicene sheets. Therefore, it is of interest when the Li ion can pass a path of approximately this length in silicene. The electric field ( $10^5$  V/m) used in this study was chosen empirically. This field cannot have a significant impact on the parameters of the electron orbits of atoms and consequently cannot make changes to widely used interatomic interaction potentials. We investigated the diffusion of lithium in the two-layer silicene with AB stacking which has a lower binding energy (−5.32 eV) than silicene with AA laying (−5.25 eV) or a monolayer silicene (−5.13 eV) [7].

The purpose of this work is to investigate the structure, kinetic, and mechanical properties of the two-layer porous silicene at its interaction with the lithium ion in constant transverse and longitudinal electric fields.

## 2. Methodology

The calculations were performed by classical molecular dynamics. Tersoff potential with the parameters of Ref. [8] was taken for representation of the interactions in silicene. The interaction between Si belonging to different sheets of silicene is described by

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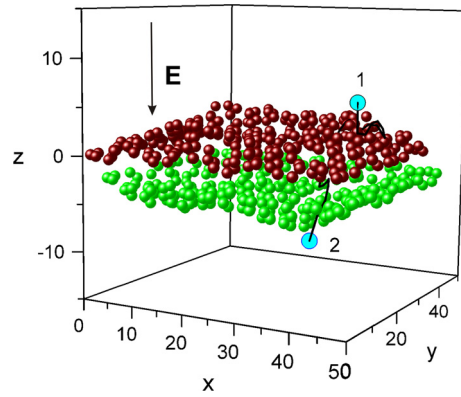
Morse potential [9]. The interaction between the  $\text{Li}^+$  ion and atoms of Si was presented by Morse potential too [10,11].

In this paper we consider the case of the  $4 \times 4$  surface reconstruction. The unit cell of a silicene structure contains 18 Si atoms. Six atoms of the unit cell are displaced by the distance of 0.074 nm perpendicular to the surface and the other Si atoms are on the same (original) plane. Such a structure is similar to an arrangement of the silicene surface observed on the Ag(111) substrate [12]. If atoms protruding above the original surface in the top-sheet of the two-layer silicene are displaced upwards such atoms of the lower sheet stayed down. Various periodic structures are observed for silicene on Ag(111) such as  $4 \times 4$ ,  $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$ ,  $(\sqrt{7} \times \sqrt{7})R19.1^\circ$ , and  $(\sqrt{13} \times \sqrt{13})R13.9^\circ$  [13–15]. Almost all experimental studies confirm that Si atoms in silicene form a buckled honeycomb lattice. We apply the  $4 \times 4$  model of silicene, since its validity was confirmed by various experimental methods including non-contact atomic force microscopy, scanning tunneling microscopy, angle-resolved photoelectron spectroscopy, and low-energy electron diffraction [12]. In addition, atomic structure of the monolayer  $4 \times 4$  silicene occupies the largest part of the surface of epitaxial silicene on the substrate Ag(111) [16]. During the entire calculation, the average height of the protrusions produced by the Si atoms in the model was kept with a good degree of accuracy. A slight difference ( $<0.005$  nm) in the height of the buckles as well as the horizontal dimensions of the reconstruction determined by different models of silicene obviously cannot greatly affect the result of the simulation. The simulation results show that the  $h_g$  gap between the silicene sheets exerts the main influence on the final result. It is the value of  $h_g$  and the electric field strength that determine the channel capacity.

The estimated concentrations of mono- and bi-vacancies in silicene obtained on Ag(111) can be quite high such as  $4.4 \times 10^{13} \text{ cm}^{-2}$  and  $5.0 \times 10^{13} \text{ cm}^{-2}$  respectively [17]. It means that there would be one defect in every  $2 \text{ nm}^2$  area. The large concentration of point defects together with easy diffusion and coalescence of vacancy defects nicely explains a low stability of silicene in experiments.

The study of the  $\text{Li}^+$  ion permeation through the pores of the Si-membranes was performed in the presence of the gap between the silicene sheets  $h_g = 0.2481$  nm. In the case of the  $\text{Li}^+$  ion movement in the flat channel under action of the longitudinal electric field the gap was  $h_g = 0.75$  nm wide. Perfect silicene sheet had a size of  $4.8 \times 4.1$  nm (taking into account the size of Si atoms) and contained 300 atoms. 9 similar defects were created approximately evenly with a displacement of 0.1–0.2 nm in each ( $x$  and  $y$ ) direction for different sheets in silicene: single vacancies, bi-vacancies, tri-vacancies, hexa-vacancies. The silicene sheet contained 291, 282, 273 and 246 atoms in each of these cases.

The study of vertical (perpendicular to the plane of the membrane)  $\text{Li}^+$  ion transport through silicene sheets was performed by 20 tests for each set of membranes. Twenty points for initial arrangement of ions were placed almost evenly over the top sheet of silicene. Each test was carried out for the new location of the ion and had duration of 1 million time steps. During this time, in most cases the ion successfully overcame the double-barrier in the form of silicene membranes containing mono- or poly-vacancies. The average time for ion to overcome silicene obstacles was determined on the basis of these tests. Only successful tests were taken into account. In the case of the horizontal ion movement two sheets of silicene contained the same set of defects and the ion was similarly moved by the longitudinal electric field intensity of  $10^5$  V/m. Initially (at  $t = 0$ ), the  $\text{Li}^+$  ion was located at coordinates  $x = 0.198$  nm,  $y = 2.245$  nm, i.e. it was slightly pushed into silicene channel. In this case, each run had duration of 1 million time steps.



**Fig. 1.** The drift of lithium ion through the bi-layer of silicene membrane with single vacancies; circle 1 shows the original location of the ion, circle 2 reflects the ion's location immediately after the passage through membrane; the arrow shows the strength vector of the applied electric field; atomic coordinates are given in Angstroms.

Securing the sheet edges of silicene creates conditions for preserving the morphology of porous silicene. The numerical solution of the motion equations was performed by the Runge–Kutta method of order 4 with the time step of  $\Delta t = 1 \times 10^{-16}$  seconds.

Self-diffusion coefficient was calculated by the mean square displacement of the atoms  $\langle [\Delta \mathbf{r}(t)]^2 \rangle$

$$D = \lim_{t \rightarrow \infty} \frac{1}{2\Gamma t} \langle [\Delta \mathbf{r}(t)]^2 \rangle, \quad (1)$$

where  $\Gamma = 3$  is dimension of the space, the  $\langle \dots \rangle$  angle brackets denote averaging over time.

The surface roughness (arithmetic mean or the profile deviation) was calculated as [18]

$$R_a = \frac{1}{N} \sum_{i=1}^N |z_i - \bar{z}|, \quad (2)$$

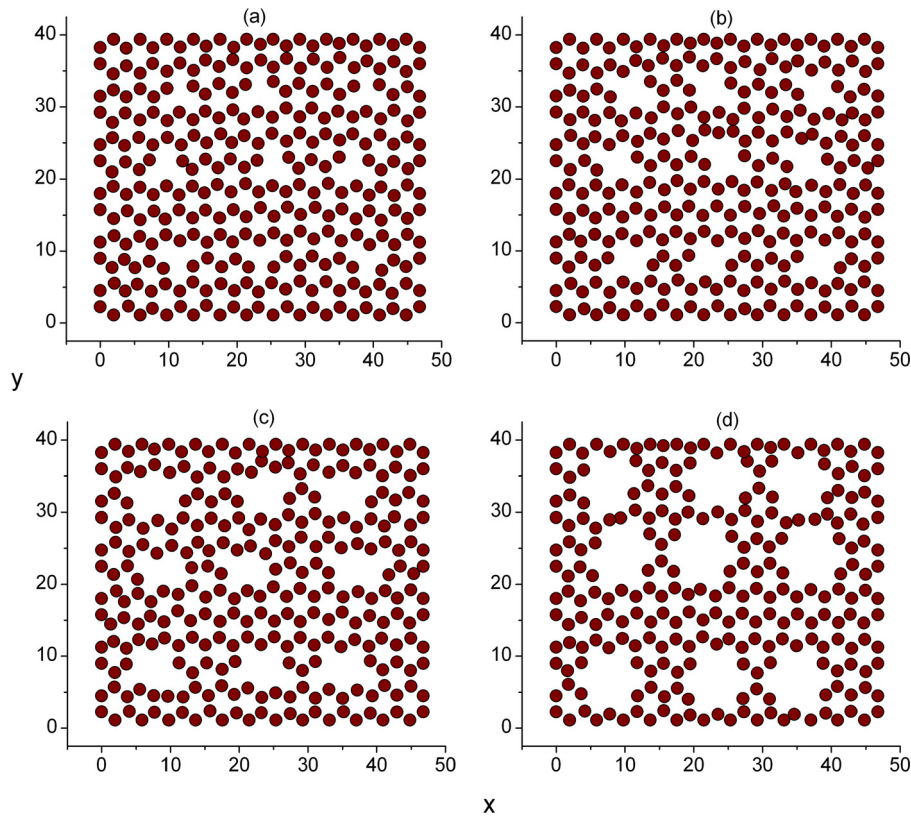
where  $N$  is the number of nodes (atoms) on the surface of silicene,  $z_i$  is the  $i$  atom displacement in the  $oz$  axial direction,  $\bar{z}$  is the average value of the coordinates for the silicene sheet, values  $z_i$  and  $\bar{z}$  are determined in the same time.

Stresses that appear in silicene were calculated according to circuit present in [19] (Eqs. (14) and (15)).

A modified LAMMPS code [20] for parallel computing in the applied MD method was used. Fragments were introduced in the program to calculate kinetic and mechanical properties of the system. The calculations were performed on a hybrid cluster calculator “Uran” at IMM UB RAS with a peak performance of 216 Tflop/s and 1864 CPU.

### 3. Results

Consider first the situation where the direction of the electric field vector is perpendicular to the plane of the silicene membrane. Suppose that in this case the pores appear to be single vacancies. Ion of lithium initially moves in the direction of the field. Fig. 1 shows ion passage through the pores of a two-layer silicene where open circles marked with numbers 1 and 2 refer to the original location of the ion and the location immediately after its overcoming a two-layer membrane respectively. The top layer of the membrane is shown in the figure by dark beads and the bottom layer is presented by lighter beads. It is evident that from place of the entrance into the upper layer to the exit point of the lower layer, i.e. in the space between the layers, the ion overcame a considerable distance. The residence time in the interlayer space in this case may be a few picoseconds. First ion diffuses over the surface



**Fig. 2.** The horizontal projections of the upper silicene membranes having pores in the form of: (a) single vacancies, (b) bi-vacancies, (c) tri-vacancies, (g) hexa-vacancies. Projections correspond to the time of 100 ps.

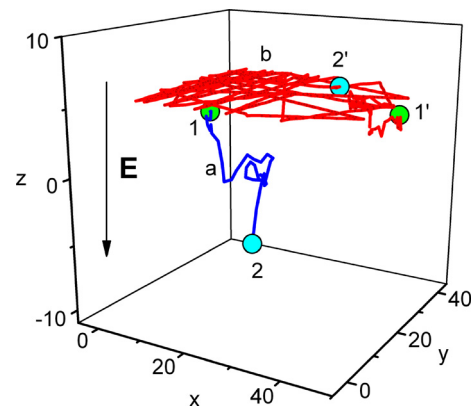
of silicene until it finds a position to enter the flat channel. Then, describing a complex trajectory, it is looking for a way out of this channel and having found a vacancy in the lower layer it leaves the channel. Replacement of defects in the sequence: a single vacancy, di-vacancy, tri-vacancy, hexa-vacancy leads to shortening of the path which ion overcomes inside the two-layer silicene and the time of overcoming these obstacles reduces.

Constructions created by nature are sometimes used in engineering. In fact, the model we use is similar to the crude model of the cell membrane. Some channels open or close in neurons and muscle cells in response to changes in the charge across the membrane plasma. Also it is possible to active transport, i.e. to pump molecules or ions through a membrane against their concentration gradient.

The horizontal projections of the upper sheets of the two-layer silicene which defects are represented by mono-, bi-, tri-, and hexa-vacancies are shown in Fig. 2. The projections are obtained after performing 1 million time steps in MD model. Vacancies of each species retained their shape except small distortions.

Starting the movement from one of the 20 points evenly distributed over the surface of silicene ion  $\text{Li}^+$  is not always able to pass through the bi-layer silicene membrane. In some cases throughout the timing (mainly for membranes with single vacancies) ion was moving along the surface of the top sheet of silicene and non-penetrating through it. An example of such a trajectory is shown by the curve “b” in Fig. 3. Curve “a” shows the trajectory when the  $\text{Li}^+$  ion after a short movement passes through the bi-layer silicene membrane. The direction of the electric field intensity is shown by the arrow.

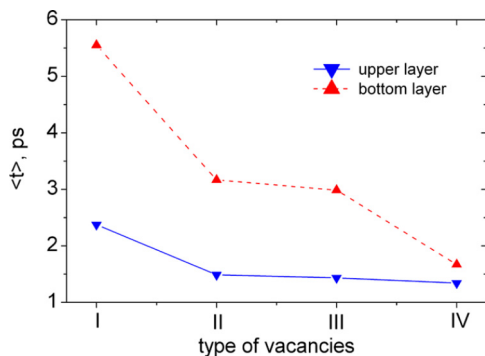
The mean time  $\langle t \rangle$  which the  $\text{Li}^+$  ion needs to overcome each of the silicene layers is shown in Fig. 4. It is seen that the  $\langle t \rangle$  time for passage of the first (upper) layer has a substantially larger value only in the case where silicene sheets contain mono-vacancies.



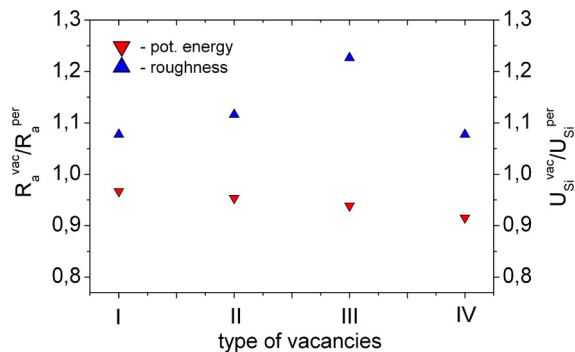
**Fig. 3.** The two trajectories (a, b) of lithium ion moving under the influence of the electric field  $E$ ; 1, 1' are the ion motion start points; 2, 2' reflect points of ion location through 100 ps; points 1, 2 refer to the “a” trajectory, 1', 2' correspond to the “b” path.

A similar trend is observed in the second (bottom) layer. The ion passage of the second layer of silicene in the presence of bi- and tri-vacancies requires much longer time than that in the presence of hexa-vacancies. At the same time the  $\langle t \rangle$  value of the interlayer ion drifts in the presence of bi-vacancies in layers is only slightly higher than that in the case of tri-vacancies presence in silicene sheets.

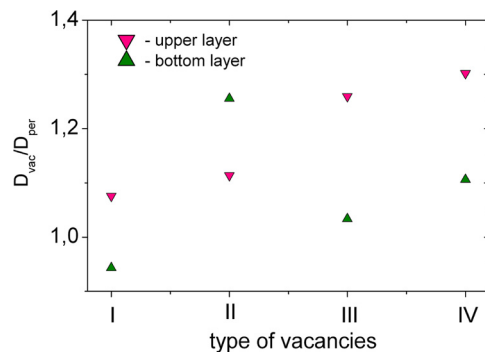
When the  $\text{Li}^+$  ion moves along the channel, it “clings” to sheets of silicene and slows down in the channel. Moreover, the  $\text{Li}^+$  ion in silicone channel easily moves in the opposite direction to the applied electric field. The  $\text{Li}^+$  ion passes through the entire length of the channel and leaves it when the gap  $h_g = 0.80$  nm and silicene is perfect or has mono- or bi-vacancies. The ratios of roughnesses and potential energies are shown in Fig. 5, where



**Fig. 4.** The mean time of the lithium ions' passing through the first and the second layer of the two-layered silicene. The numbers on the  $x$ -axis denote the type of defects in the membranes: I mono-vacancy, II bi-vacancies, III tri-vacancies, IV hexa-vacancies.



**Fig. 5.** The ratio of roughness and potential energy of porous silicene to the values of perfect silicene during the lithium longitudinal movement in the channel. The numerical designation is similar to that in Fig. 4.

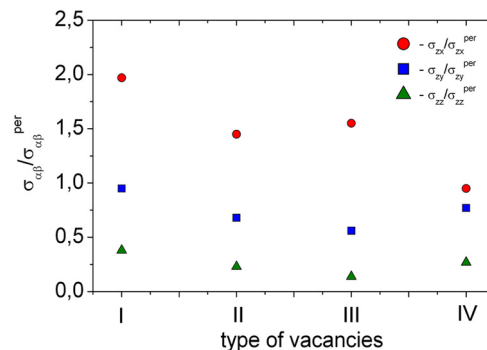


**Fig. 6.** The ratio of self-diffusion coefficients of Si atoms in the sheets of porous silicene to the corresponding characteristics of the perfect silicene with lithium longitudinal movement in the channel. The numerical designation is similar to that in Fig. 4.

the corresponding characteristics with the upper indexes “vac” and “per” designate the defective and perfect silicene respectively and are determined at the longitudinal movement of lithium ion between silicene sheets with the gap of 0.75 nm.

With increasing pore size potential energy of the system increases while the average roughness passes through the maximum which falls on the system III. Thus borders with tri-vacancies are the most vulnerable to displacements perpendicular to the plane of each membrane.

Fig. 6 reflects similar relative characteristic for self-diffusion coefficient of Si atoms in the two identical sheets of silicene with the gap between the sheets of 0.75 nm. In almost all cases, the ratio is  $D_{vac}/D_{per} > 1$ , i.e. the mobility of Si atoms in the membranes with pores is greater than that in the perfect silicene sheets.



**Fig. 7.** Change of stresses acting in the plane of silicene sheets in cases of appearance of mono- and poly-vacancies in them. The numerical designation is similar to that in Fig. 4.

With exception of the lower membrane with single vacancies for which mobility of Si atoms decreases due to changes in its relief and the reduction of the force of interaction with  $Li^+$  ion drifting in the space between silicene sheets. The peak mobility for the lower sheet of silicene corresponds to the membrane with bi-vacancies. In this case, the ion passing along the lower membrane transmits Si atoms of more energy due to frequent collisions with boundaries of bi-vacancy atoms comparing to other cases under consideration. The ion “glides” along the surface of this membrane in much shorter time.

In connection with the questions considered here, it is important to know the stresses appearing in the sheets of silicene between which the lithium ion moves. The average stresses appearing in this process in the plane of the perfect silicene sheets are:  $\sigma_{zx}^{per} = 0.22$  GPa,  $\sigma_{zy}^{per} = 2.38$  GPa,  $\sigma_{zz}^{per} = 0.75$  GPa. The strongest stress ( $\sigma_{zy}^{per}$ ) appears as a result of the action of the force directed perpendicularly to the electric field strength vector. Fig. 7 shows the relative average stresses acting in defective silicene sheets when lithium ion moves between them. It can be seen that as a rule the weakest stress ( $\sigma_{zx}$ ) in defective silicene is amplified and more significant stresses ( $\sigma_{zy}$  and  $\sigma_{zz}$ ) are weakened. A particularly strong decrease is observed for the  $\sigma_{zz}$  stress which is associated with an increase in the freedom of the ion movement in the  $oz$  direction due to the presence of poly-vacancies.

#### 4. Discussion

Defects in the silicene sheet appear significantly easier than in graphene. Defects in the graphene do not lead to a loss of stability of the system even in the presence of lithium ion moving in an electric field [21]. Really, systematic silicon modification may allow creation of new anode materials. The composite graphene–Si anode demonstrated high and stable values of reversible capacity of about 1000 mAh/g after 100 cycles at the current equal to 500 mA/g [22]. Comparing with other carbon matrices graphene can be easily folded or deformed to create 3D networks that can serve as structures for connection of graphite and silicon [23].

However, when using silicene together with graphene in a composite anode, one should take into account not only the difference in their mechanical and electrical properties but also the interaction of these dissimilar materials with lithium ions. Silicene is a much less durable material than graphene [24]. Its stability, especially when silicene has a large number of defects with respect to friction and the movement of lithium ions around it under the influence of electric field, is not high. The  $Li^+$  ion movement between the sheets of silicene requires application of a much stronger electric field ( $10^5$  V/m) than the field ( $10^3$  V/m), which is needed to move it in a flat channel formed by sheets of graphene [25]. Movement of lithium ions is more controlled when they

move along the graphene channel than silicene analogue, in which the ion trajectory covers a large area of the silicene sheet [26]. In the case of silicene the  $\text{Li}^+$  ion inputs in a flat channel easier, but the ion usually gets stuck in the silicene channel even if the channel has sufficiently large value of  $h_g$  and significantly higher values of the applied electric field are used.

The average stress of the zigzag direction (0.22 GPa) appearing in perfect silicene does not exceed 5% of the stress limit which is installed in silicene under uniaxial tension [27]. However, in the presence of mono-vacancies this stress approaches 13% of the corresponding stress  $\sigma_{zx}$ . We cannot make such a comparison if there are larger poly-vacancies in silicene because of the lack of data on the ultimate stretching. Note that the  $\sigma_{zx}$  calculated value has some decrease for silicene with poly-vacancies. Stresses  $\sigma_{zy}$  and  $\sigma_{zz}$  initially decrease with increasing defect size, but for silicene with hexa-vacancy they increase. At the same time, the  $\sigma_{zx}$  stress in the case of the presence of hexa-vacancies in silicene decreases substantially, compensating for the increase in  $\sigma_{zy}$  and  $\sigma_{zz}$ . Redistribution of stresses in silicene containing hexa-vacancies is associated with an amplification in the symmetry of defects and a change in the role of various Si–Si bonds. The  $\sigma_{zy}$  stress caused by the action of forces directed parallel to the plane of silicene and perpendicular to the electric field strength vector is the most significant among the other stress components acting in the plane of the silicene sheet. As expected, the creation of vacancy defects leads to the strongest decrease in the stress caused by the action of vertical forces. For all types of defects, the stress in silicene is more than 2 times lower than for the pristine silicene. Thus, a change in the mechanical properties of the defective silicene is not critical for its use as an anode material.

## 5. Conclusion

The passage of lithium ions through a two-layer porous silicene and the motion of the ion in a flat channel formed by sheets of porous silicene in the presence of an electric field have been studied. Mean transit time of the ion through the silicene membrane in transverse electric field is reduced with an increase in the pore size of silicene. Under the influence of the longitudinal electric field the  $\text{Li}^+$  ion performs complicated oscillating movement in the space between silicene membranes and is experiencing difficulty to exit from the gap bounded by the sheets of silicene. The simulation showed that bi-vacancies in silicene are more stable than tri- and hexa-vacancies. They retain their shape with frequent ion strikes on boundaries of the pores, at much higher values of  $D$  coefficient than other poly-vacancies. The presence of sufficiently large number of mono- and bi-vacancies in silicene allows monitoring of the charging/discharging process of electrode. However coarsening of the size of defects, i.e. replacement of mono- and bi-vacancies on tri- and hexa-vacancies makes corresponding processes uncontrollable. The  $\sigma_{zx}$  stress caused by the electrostatic force  $e \cdot \mathbf{E}$  is greatly enhanced when the lithium ion moves in a flat channel formed by defective silicene sheets. There is a redistribution of the stresses existing during the motion of the lithium ion in silicene when the symmetry of defect coincides with the symmetry of the two-dimensional structure. The most significant stress is produced by transverse forces acting parallel to the plane of silicene and perpendicular to the electric field strength vector. The results of the present study may be useful in the development of the silicene anode design for lithium-ion batteries.

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