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SURFACE PHYSICS AND THIN FILMS =

Defect Silicene and Graphene as Applied to the Anode of Lithium-Ion Batteries: Numerical Experiment

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Abstract—Mechanical properties and stability of two layers of defect silicene supported by graphene sheets, between which the lithium ion passes under an electrostatic field, are studied by the molecular dynamics method. Defects are mono-, di-, tri-, and hexavacansies. Graphene and silicene edges are rigidly fixed. Graphene sheets contacting with silicene take a convex shape, deflecting outward. Mono- and divacancies in silicene tend to a size decrease; larger vacancies exhibit better stability. The ion motion control using an electric field becomes possible only using perfect silicene or silicene with mono- and divacancies. The ion penetrated through larger defects, and its motion in the silicene channel becomes uncontrolled. When the ion moves in the channel, the most strong stress spikes appear in silicene containing monovacancies. In the case of fixed edges, perfect silicene intercalated with a lithium ion is inclined to accumulate larger stresses than silicene containing defects.

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1. INTRODUCTION

The field of application of silicene with honeycomb structure is extensive. For example, silicene is applicable to fabricate ultrasensitive chemical sensors or electronic "noses," biological markers, to improve solar cells and fuel cells, including those for hydrogen storage [1-4].

Free silicene has electronic properties similar to those of graphene. However, for now, it manages to synthesize silicene-like structures only on various substrates whose surface structure strongly changes silicene properties. As a result, the electronic structure and properties can differ significantly from those theoretically predicted for free silicene. To achieve expected electronic properties, silicene should be stabilized using surfaces very weakly interacting with it. Due to the reactive activity of Si atoms, it is very difficult to select such surfaces. However, it can be attempted to strengthen silicene by supporting it by graphene sheets. It is assumed that graphene having unique electronic properties will not significantly degrade silicene properties. There is an opinion [5] that two-layer silicene retention between planar graphene sheets will cause flattening of sponge silicon layers, i.e., will impart a small bond bending in the local environment of Si atoms, which is energetically unfavorable in vacuum. Such a statement is not quite correct. In fact, free single-layer graphene is no longer an ideal plane, but is susceptible to corrugation according to theoretical Peierls [6] and Landau [7] predictions. Therefore, silicene supported by graphene should also be bent. Furthermore, to make feasible the graphene support, the closest distance between graphene and silicene should be small, i.e., comparable to the distance between nearest neighbors in silicene. However, the interaction between graphene and silicene in this case will not be weak, i.e., will not have a Van der Waals form, as assumed in [5]. In the case of the chemical reaction between silicon and carbon with the formation of silicon carbide, the interaction between Si atoms and C is even stronger than between atoms in silicon. Therefore, as silicene and graphene sheets approach to short distances, the Si-C interaction will not be weak. In the case of the strong interaction between Si and C atoms, the shape of each sheet will adapt to the adjacent sheet shape. However, since interatomic bonds in silicene are significantly longer than in graphene, the adjacency between graphene and silicene sheets cannot be tight over the whole area. In other words, the figured floral structure of silicene such as it takes on the Ag(111) substrate [8] not only should be destructed when contacting with graphene, but can be deepened even more. This means that the vertical displacement of Si atoms will be enhanced in the case of silicene support by a graphene sheets. At the same time, incomplete graphene adjacency to silicene, caused by bond length mismatch, will weaken the interaction between these sheets. Therefore, the silicene sheet will not exactly reproduce the graphene sheet shape.

It is clear that the relief of silicene enclosed between graphene sheets will be enhanced, if silicene contains mono- and polyvacancies. This is due to Si-Si bond weakening in defect silicene. As a practical matter, silicene strengthening by graphene is of interest when using bilayer silicene as an anode of the lithium-ion battery. It is known that the use of bilayer silicene decreases the change in the silicon anode volume from 400 to 24%, which occurs during intercalation/deintercalation of Li⁺ ions [9]. This radically solves the problem of the use of silicon in portable energy accumulation and storage devices. Therefore, it appears attractive to use graphene-strengthened silicene in power electrochemical elements. Defects distributed in actual silicene (mono- and polyvacancies) have an effect on the silicene-graphene anode operability. First of all, this is concerned with transport properties of lithium ions.

The objective of this work is to study to what extent will change the migratory ability of the lithium ion enclosed between fragments of bilayer silicene supported on the outside by graphene sheets in the cases, where silicene contains a large number of mono- or polyvacancies.

2. NUMERICAL MODEL

Interatomic Si–Si, Si–C, and C–C interactions were presented by the Tersoff many-body potential [10]

$$V_{ij} = f_C(r_{ij}) [A_{ij} \exp(-\lambda^{(1)} r_{ij}) - Bb_{ij} \exp(-\lambda^{(2)} r_{ij})], \quad (1)$$

where

$$f_{C}(r_{ij}) = \begin{cases} 1, & r_{ij} < R^{(1)}, \\ \frac{1}{2} + \frac{1}{2} \cos \frac{\pi(r_{ij} - R^{(1)})}{(R^{(2)} - R^{(1)})}, & R^{(1)} < r_{ij} < R^{(2)}, \\ 0, & r_{ij} > R^{(2)}, \\ b_{ij} = (1 + \beta^{n} \xi_{ij}^{n_{i}})^{-1/(2n)}, \\ \xi_{ij} = \sum_{k \neq i, j} f_{C}(r_{ij})g(\theta_{ijk}), \\ g(\theta_{ijk}) = 1 + \frac{c^{2}}{d^{2}} - \frac{c^{2}}{[d^{2} + (h - \cos \theta_{ijk})^{2}]}, \\ \lambda_{ij}^{(k)} = (\lambda_{i}^{(k)} + \lambda_{j}^{(k)})/2, \quad A_{ij} = (A_{i}A_{j})^{1/2}, \\ B_{ij} = (B_{i}B_{j})^{1/2}, \\ R_{ij}^{(1)} = (R_{i}^{(1)}R_{j}^{(1)})^{1/2}, \quad R_{ij}^{(2)} = (R_{i}^{(2)}R_{j}^{(2)})^{1/2}. \end{cases}$$
(2)

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Here, b_{ij} is the many-body bond order parameter describing the bond energy formation (attractive part of the potential V_{ij}) in the case of the local atomic arrangement due to the presence of other neighboring atoms, ξ is the effective coordination number, $g(\theta_{ijk})$ is the function of the angle between r_{ij} and r_{ik} , stabilizing the structure; subscripts i, j, k denote carbon or silicon atoms, r_{ij} is the i-j bond length, and θ_{ijk} is the angle between i-j and j-k bonds.

The Tersoff potential parameters for silicon and carbon, listed in the table were taken from [11]. The potential function parameters $\lambda_{ij}^{(k)}$, A_{ij} , B_{ij} , $R_{ij}^{(k)}$ describing the interaction between Si and C atoms were calculated using arithmetic and geometric means (see Eq. (2)). The procedure of fitting other parameters when using the original Tersoff potential is described in [12]. The Tersoff potential has a good transferability for bond orbitals; the parameters fitted to sp^3 -hybridization can be used to describe the interaction in materials with sp^2 -hybridization [13].

The interaction between Si atoms belonging to different silicene sheets was described by the Morse potential [14]

$$\Phi(r) = D_e[\exp\{-2\alpha(r - r_e)\} - 2\exp\{-\alpha(r - r_e)\}], (3)$$

where D_e is the potential well depth, α is the rigidity parameter, and r_e is the equilibrium bond length. The Morse potential was also used to represent the interaction between the Li⁺ ion and Si and C atoms. The parameters of this potential (see the table) were determined using the corresponding data for describing the Li–Li [14], Si–Si [15], and C–C [16] interactions.

If the Morse potential parameters for representing the interactions between A- and B-type atoms, the parameters of AB interactions are determined using the simple interpolation relations [15]

$$D_{e}^{AB} = (D_{A}D_{B})^{1/2},$$

$$\alpha^{(AB)} = \frac{1}{2}(\alpha_{A} + \alpha_{B}),$$

$$r_{e}^{AB} = (r_{e}^{A}r_{e}^{B})^{1/2}.$$
(4)

The Morse potential parameters used in the present study are listed in the table.

The model under consideration implies the 4 × 4 surface reconstruction. The unit cell this rhombshaped silicene structure contains 18 Si atoms. Six Si atoms of the unit cell are displaced by 0.074 nm normally to the surface; other Si atoms are on the same (initial) plane. The initial structure of the silicene sheet was close to the silicene surface observed on the Ag(111) substrate [8]. If Si atoms protruding above the initial surface in the upper sheet of bilayer silicene are displaced upward, such atoms in the lower sheet are displaced downward. We performed a number of calculations for choosing the optimum distance h_g between silicene sheets. The calculations were started Tersoff potential parameters

Interaction		A, eV B, eV		λ_1, nm^{-1}	λ_2, nm^{-1}		λ_3, nm^{-1}	п
Si—Si		1830.8	30.8 471.18 2.4799 1.7322		322	0	0.78734	
C–C		1393.6	346.7	3.4899	2.2119		0	0.72751
		С		d	<i>R</i> ⁽¹⁾ , nm	<i>R</i> ⁽²⁾ , nm	β	h
Si—Si		1.0039×10^5		16.217	0.27	0.30	1.1×10^{-6}	-0.59825
C–C		3.8049×10^4		4.384	0.18	0.21	1.5724×10^{-7}	-0.57058
Morse potential parameters								
$D_e^{\mathrm{Si-Si}}$, eV	α^{Si-Si}, nm^{-1}	$r_e^{\text{Si-Si}}$, nm	$D_e^{\text{Li-Si}}$, eV	α^{Li-Si} , nm ⁻¹	$r_e^{\text{Li-Si}}$, nm	$D_e^{\text{Li-C}}$, eV	$\alpha^{\text{Li-C}}, nm^{-1}$	$r_e^{\text{Li-C}}$, nm
0.2274	15.390	0.44992	0.30932	11.6445	0.36739	1.25851	17.0745	0.20647

Tersoff and Morse potential parameters for representing the Si-Si, C-C, Si-C, Li-Si, and Li-C interaction

from a spacing of 0.60 nm and finished by the value $h_g = 0.80$ nm with step $\Delta h_g = 0.05$ nm. The plane channel formed of perfect silicene sheets supported on the outside by graphene sheets was simulated. It was found that beginning from the distance $h_g = 0.75$ nm, the Li⁺ ion passes between silicene sheets along the entire channel length. The high electrode capacitance is achievable when electrolyte ions rapidly move so that the *D* ion self-diffusion coefficient would be in the range of $10^{-14}-10^{-17}$ m²/s [17]. At spacing $h_g = 0.75$ nm, the lithium ion coefficient *D* falls within this interval, where the electric field strength is 10^5 V/m. This distance significantly exceeds 0.2481 nm between bilayer silicene sheets with *AB* packing, obtained from density functional theory calculations [5].

Perfect silicene sheets (Fig. 1a) containing 300 atoms each were rectangular shaped (4.7 \times 4.0 nm; 12 atoms were arranged along each sheet edge). Brighter atoms protrude above the plane formed by darker atoms. Nine mono- and polyvacancies were arranged approximately uniformly over the silicene sheet area: therefore, the number of Si atoms in each sheet was 291, 282, 273, and 246 for sheets with mono-, di-, tri-, and hexavacancies, respectively. The initial configuration of the silicene sheet containing divacancies is shown in Fig. 1b. A dc electric field with a strength of 10^5 V/m accelerated the Li⁺ ion along the x axis oriented in the "zigzag" direction of graphene sheet. Silicene sheets were arranged according to the Bernal stacking (AVAV...) in the exactly similar way as in bulk graphite. Graphene sheets were placed in parallel to silicene sheets outside the channel; therewith, the distance between silicene and graphene sheets was the same as in [5], i.e., 0.222 nm. Frontal edges of graphene and silicene sheets were superposed. Each rectangular graphene sheet contained 820 atoms; along each of its edges, 20 C atoms were arranged. The primary ion position corresponded to the height $h_g/2$. At the initial time (at t = 0), the ion was at the point with coordinates x = 0.198 nm, y = 2.245 nm, i.e., it was slightly pushed to the silicene channel approximately at the sheet middle.

The equations of motion were numerically solved by the fourth-order Runge–Kutta method with time step $\Delta t = 1 \times 10^{-16}$ s. The duration of each calculation with spacing h_g was 10^6 of time steps. In the calculations, the code we modified for parallel molecular dynamics method calculations (LAMMPS) [18] was used. The fragments of the program for calculating kinetic and mechanical properties of the system were introduced. The calculations were performed using the "URAN" cluster-type hybrid computer at the Krasovskii Institute of Mathematics and Mechanics,



Fig. 1. Configurations of (a) perfect silicene and (b) silicene with divacancies. The brighter images of atoms are elevated over the plane formed by other (dark) atoms by 0.074 nm.

Ural Branch of the Russian Academy of Sciences, Yekaterinburg, with a peak processing speed of 216 Tflop/s and 1864 CPU.

To calculate stresses arising in graphene, the graphene sheet was divided into elementary areas. The stresses $\sigma_{u\alpha}(l)$ caused by forces in the $\alpha = x, y, z$ direction are calculated for each *l*-th area with *u* orientation. In these calculations, the products of projections

of atomic velocities and projections of forces f_{ij}^{α} acting on the *l*-th area from the side of other atoms, if corresponding conditions are satisfied [19],

$$\sigma_{u\alpha}(l) = \left\langle \sum_{i}^{k} \frac{1}{\Omega} (m \mathbf{v}_{u}^{i} \mathbf{v}_{\alpha}^{i}) \right\rangle + \frac{1}{S_{l}} \left\langle \sum_{i}^{k} \sum_{j \neq 1}^{(u_{i} \leq u, u_{j} \geq u)} (f_{ij}^{\alpha}) \right\rangle.$$
(5)

Here, k is the number of atoms on the *l*-th area, Ω is

the volume per atom, *m* is the atom mass, v_{α}^{i} is the α -projection of the *i*-th atom velocity, and S_{l} is the *l*-th area. The conditions of summation over *j* in the last sum of expression (5) are reflected in both the lower and upper bounds of the sum; the force arising during the interaction of atoms *i* and *j* passes through the *l*-th area; u_{i} is the current coordinate of atom *i*; in the upper bound of the sum, *u* is the coordinate of the point of contact of the straight line passing through the centers of atoms *i* and *j* with the *l*-th area. Compressive stresses in such a definition can have "plus" or "minus" signs according to the directions of forces f_{J}^{i} . This is the difference of the microscopic stress $\sigma_{uJ}(l)$ from the macroscopic compressive stress $\overline{\sigma}_{J} < 0$. The total stresses in the graphene plane were determined by summing corresponding elementary stresses [20],

$$\sigma_{zJ} = \sum_{l=1}^{N_l} \sigma_J^z(l), \qquad (6)$$

where N_l is the number of elementary areas when dividing the graphene sheet in the chosen direction.

3. CALCULATION RESULTS

The Li⁺ ion trajectory in the silicene–graphene channel formed by monovacancy-saturated silicene is schematically shown in Fig. 2. The initial and final points of the ion are denoted by numbers 1 and 2, respectively. When moving in the channel, the Li⁺ ion executes strong vertical pulsations. In the central region of the lower sheet, the moving ion strongly bends the silicene sheet. As a result of the hard contact of silicene with graphene, the ion almost instantly returns to the silicene channel at the contact point and continues its translatory-oscillatory motion along the electric field. At a certain distance from the channel output, the ion decelerates its translational motion, executing frequent vertical vibrations. Eventually, it stops near the channel output and moves upward, passing near the edge of the upper silicene sheet, hits



Fig. 2. Lithium ion trajectory in the silicene–graphene channel in the case where defects in silicene are presented by monovacancies. (1) and (2) are initial and final trajectory points, respectively.

the edge of the upper graphene sheet and, having slightly changed its trajectory, escapes from the device. The ion path shown in the figure took 280000 time steps (or 28 ps). When defects in silicene were divacancies, the ion passed the first part of the path for a very long time; however, it passed through the output along the straight trajectory starting from the first part of the silicene sheet. The channel passage took 68 ps. When the channel supported by graphene was formed by silicene filled with trivacancies and hexavacancies, the Li⁺ ion could not pass throughout the channel. It mostly walked outside the channel, was within it for a very short time, emerged through the upper or lower silicene sheet, and no longer arrived at the channel. From the motion start until the time point when the ion finally left the channel, 26 ps elapsed in the case of trivacancies and 13 ps in the case where hexavacancies were defects. Thus, the ion trajectory control was fully lost if silicene contained tri- or hexavacancies.

The interaction between graphene and silicene externally manifested itself as the convex graphene shape with outward convexity in all cases under consideration. Figure 3 shows the configuration of the plane silicene–graphene channel formed by silicene with monovacancies, immediately after passing the Li^+ ion through the channel output, i.e., at the time point of 28 ps. We can see that graphene sheets cannot be approximated by a plane. Silicene is more appropriate for this approximation; however, its sheets are appreciably rough.

The defect dynamics is traced by horizontal projections of silicene sheets. Figure 4 shows the projections of the upper silicene sheet containing nine divacancies at different time points. After the lapse of 100 ps, the number of defects in silicene remained the same as at



Fig. 3. Configuration of the plane channel formed by defect silicene and graphene, related to the time point of 28 ps corresponding to lithium ion exit from the channel. Defects in silicene are presented by monovacancies.

the initial time, i.e., 9. However, not all defects retained their primary shape. For example, the defect in the left upper corner eventually transformed into an ellipse formed by eight Si atoms. In this case, its area decreased. As a whole, silicene retained its cellular structure filled with equally spaced defects. Similar defect dynamics is traced for silicene sheets filled with monovacancies. By the time of 100 ps, three monovacancies appeared lost due to the redistribution of Si atoms, resulting in defect overgrowth. The number of larger defects (tri- and hexavacancies) was retained to the calculation end. The defect area reduced in the case of trivacancies and remained almost unchanged for hexavacancies. Thus, minor defects in silicene supported by graphene tend to self-removal or at least to size reduction. At the same time, large defects, such as hexavacancies, retain shape and sizes for a significantly longer time.

Stable operation of the considered electrode element is provided by its mechanical strength. In this respect, the silicene device part is most critical. Figure 5 shows the distribution of principal stresses (σ_{zx} , σ_{zy} , σ_{zz}) in silicene over elementary areas extended along the electric field, i.e., along the x axis, calculated for the lower silicene sheet. The behavior of these characteristics for the upper silicene sheet is similar in many respects. The functions $\sigma_{\alpha\beta}(y)$ are mostly oscillating and signalternating. It is characteristic that the stresses σ_{zx} , σ_{zy} σ_{zz} arising in elementary areas are values of the same order. This is the main difference from the stress distribution in silicene sheets during Li⁺ ion drift between them without support of graphene sheets, where σ_{zz} stresses obviously dominated. Thus, the graphene support leads to a relatively uniform stress distribution in silicene. Comparing the stresses in silicene with various vacancy types (curves 1-4), we can see that an increase in the defect size do not unambiguously enhance stresses in silicene, at least for σ_{zx} and σ_{zy} . Among all dependences shown in the figure, the curves corresponding to silicene with monovacancies are distinguished. The presence of monovacancies in silicene causes the strongest surges in all three dependences $\sigma_{\alpha\beta}(y)$. These surges are at the values of y corresponding to the central part of the silicene channel, i.e., the region passed by the Li⁺ ion. The Li⁺ ion passage through the hexavacancy in silicene can also be accompanied by significant stresses; in this case, the stresses caused by horizontal forces (σ_{zx} , σ_{zy}) appear even slightly higher than the stress caused by vertical forces (σ_{zz}). In the presence of divacancies, silicene exhibits low and most steady stresses among all cases. Therefore, it can be expected that divacancies in silicene as are most abundant defects in graphene.

Figure 6 compares the total (over the entire sheet) average stresses in defect-free silicene and silicene containing various vacancies. The stresses were calculated throughout the time of the Li⁺ ion residence between silicene sheets. In all cases, σ_{zy} are the most significant stresses. As a rule, all stresses are more significant in defect-free silicene than in silicene containing vacancies or polyvacancies. Silicene sheets containing trivacancies exhibit the lowest in magnitude stresses σ_{zy} and σ_{zz} ; the least stress σ_{zx} is characteristic of the silicene sheet with hexavacancies. The strongest effect of the Li⁺ ion on the defect-free silicene sheet is associated with limited possibilities of changing the bond lengths in it.

4. RESULTS AND DISCUSSION

The present study was initiated with the selection of the interaction potentials adequately reproducing the simulated system behavior. The Brenner potential [21] complemented by the procedure eliminating the effect of uncompensated torques arising at graphene sites [22] is currently often used to simulate interactions in graphene [23, 24]. However, the use of this potential for describing the force field in supporting graphene in the model under consideration led the unexpected effect of pairwise layering and turning Si + C pairs almost perpendicular to each other using the Morse potential to describe the interaction between Si atoms belonging to different silicene sheets, or a simple turn of the entire structure, which prevents the directed motion of the Li⁺ ion, when the interaction between silicene sheets was described by the Tersoff potential. The use of the advanced Tersoff potential [25] to describe all interaction types in the system caused a rotation of the system as a whole by 45°, strong deformation of graphene and silicene, and an inward bend of sheet edges. This gave no way of studying the directed Li⁺ ion drift. The main disadvantage of all preliminarily used electrode structures was noticeable



Fig. 4. Projections of the upper silicene sheet containing divacancies, related to various time points.

damage of the silicene structure, which was detected by sheet projections onto the horizontal plane. Therefore, the study was performed with fixed edges of both graphene and silicene, i.e., the atomic motion at edges was frozen. The Tersoff potential was used to represent intrasheet Si–Si, C–C, and Si–C interactions [10, 11]; the Morse potential was used for intersheet Si–Si interactions [14–16]. The model corresponds to the actual situation where graphene supporting the silicene sheet is fixed on a rigid framework, and two such structures approach each other forming a plane channel between silicene sheets. In this case, graphene almost does not prevent the interaction of the framework with silicene.



Fig. 5. Stresses (a) σ_{zx} , (b) σ_{zy} , (c) σ_{zz} in the plane of the lower silicene sheet containing various defects: (1) monovacancies, (2) divacancies, (3) trivacancies, and (4) hexavacancies.

We showed that the used electrode design is quite stable to the Li^+ ion intercalation/deintercalation processes. Graphene and silicene sheets exhibit high flexibility and are not destructed being subjected to significant deformations when ion moving in the channel. Due to the interaction with Si atoms protruded from the silicene sheet and faced to graphene, the graphene sheet (both upper and lower) was bent outward. It is worth noting that the structure of silicene modified by vacancies, observed in the horizontal plane, was completely retained during the calculation, which is of great importance in the electrode fabrication technology.

Recently, interest has grown in the development of silicene electrodes. In [9], based on quantummechanical calculations, the energy aspect of Li^+ ion intercalation into freely standing silicene was studied. It was shown that the Li^+ ion has a rather low barrier (<0.6 eV) for silicene diffusion. In [26], a higher



Fig. 6. Total stresses (1) σ_{zx} , (2) σ_{zy} , (3) σ_{zz} accumulated by the lower sheet of perfect and defect silicene. In the horizontal axis: (0) silicene without defects, (I) silicene containing monovacancies, (II) divacancies, (III) trivacancies, (IV) hexavacancies.

(0.88 eV) energy barrier for lithium intercalation into silicene and a corresponding very low self-diffusion coefficient for lithium $(10^{-23} \text{ m}^2/\text{s})$ were predicted. The most stable place for Li atom adsorption is the site over the hexagonal silicene ring center. Two-dimensional silicene–graphene structures, as their three-dimensional analogues [27], can be successfully used in lithium-ion energy generation and storage devices. However, strongly wrinkled silicene is thermodynamically unstable during repeating lithization and delithization cycles.

5. CONCLUSIONS

The replacement of the graphite anode with a silicon analogue is necessary for the transition from the theoretical power of 372 mA h/g to a power of 4200 mA h/g. The major difficulty to achieve this goal when using bulk silicon is a significant change in the Si anode volume during lithization/delithization processes, which causes electrode disintegration, electrical contact failure, and eventually to an abrupt decrease in the capacitance. Efficient suppression of the volume change, hence, capacitance retention can be achieved by using very thin silicon films, including silicene. The use of defect silicene in the anode structure impairs the kinetics, reducing the efficiency of its operation. Fast transport of lithium ions in the thinfilm Si anode is an important factor for achieving fast Li⁺ intercalation and a significant electrode capacitance. The use of strongly defect silicene supported by graphene is possible when fixing edges (e.g., by attaching them to a rigid framework). We showed that the presence of a large number of mono- and divacancies in silicene makes it possible to control electrode charging/discharging processes. However, an increase in the defect size, i.e., the replacement of mono- and divacancies with tri- and hexavacancies makes the corresponding processes uncontrollable, hence, makes the anode inapplicable. The proposed silicene anode structure with a graphene cladding makes it possible to maintain the electrode functionality in the presence of a large number of small defects in silicene. The results obtained can find application when designing the Si anode of lithium-ion batteries with high capacitance and fast charging.

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