

GRAPHANE: DISCRETE BREATHERS FOR DEHYDROGENATION

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Abstract. Clusters of discrete breathers in fully hydrogenated graphene (also called graphane) are studied by means of molecular dynamics simulation. The energy exchange between gap discrete breathers is studied for clusters composed of two and three discrete breathers. It is shown that difference in the initial amplitude or in the initial vibration phase of discrete breathers affect the energy exchange between them. It is shown that the life time of single discrete breather in thermal equilibrium at 50 K is of order of 10 ps.

Keywords: nonlinear dynamics; discrete breather; intrinsic localized mode; graphene; graphane; dehydrogenation.

1. Introduction.

Graphene, first stable two dimensional (2D) material ever isolated, with its unique mechanical, electronic, thermal and optical properties has many potential applications. Graphene has extremely high specific surface area, low weight, high strength and it is chemically inert, which altogether makes it a very promising material for hydrogen storage. Hydrogen is an ideal energy carrier which is considered to be used as a fuel for future transport vehicles. Materials that interact with hydrogen, therefore, are important to study. The physisorption and chemisorption of hydrogen on materials with a high specific surface area is a great challenge nowadays.

Numerous studies were devoted to the hydrogenation of carbon nanotubes (CNTs) [1-3]. The main difference between CNTs and high surface area graphite is the curvature of the graphene sheets and the cavity inside the tube. The adsorption potential of 9 kJ mol^{-1} (0.093 eV) for hydrogen molecules inside (13, 0) zigzag CNTs with a diameter of 1.018 nm at 50 K was shown which is about 25% higher than the flat surface of graphite. The investigation of hydrogen absorption inside CNTs has shown that it is energetically more favorable for hydrogen atoms to recombine and form molecules [2]. A large variety of different nanostructured carbon samples have been investigated using a high-pressure microbalance [4, 5] at 77 K, electrochemical galvanostatic measurements at room temperature [6-9], and volumetric (mass flow) gas phase measurements at 77 K. From adsorption–desorption experiments, it is evident that reversible physisorption takes place with all samples. To summarize, the reversible hydrogen sorption process is based on physisorption. The amount of adsorbed hydrogen is proportional to the surface area of the nanostructured carbon sample. Together with the maximum specific surface area of carbon ($1315 \text{ m}^2 \text{ g}^{-1}$), the maximum

measured absorption capacity of the nanostructured material is 2 mass%. Several works showed the great importance of various carbon nanostructures, including graphene, for hydrogen storage [10-12]. Despite a plenty of works, the mechanisms of hydrogen desorption are still unknown.

Fully hydrogenated graphene is called graphane. The study of linear and nonlinear dynamics of graphane lattice can shed light on the basic physics of dehydrogenation. Atomistic simulations are having an increasing impact not only on the description of physical properties of known materials, but also on the prediction of novel structures and reaction paths. It was already shown by molecular dynamics simulations that a large difference in atomic weights of hydrogen and carbon leads to the appearance of a wide gap in the phonon band and, as a consequence, to the existence of nonlinear excitations called gap discrete breathers (DBs) or intrinsic localized modes [13-16] in graphane. These DBs are able to localize a large amount of energy so as to probably play an important role in overcoming the potential barrier of hydrogen desorption. DBs are spatially localized vibrational modes of large amplitude in nonlinear defect-free lattices, described theoretically for the first time three decades ago [17]. Since then, the role of DBs has been extensively discussed in relation to many physical systems [14-18]. The hypothesis proposed in the present work is that gap DBs can play an important role in the dehydrogenation of graphane. Earlier, existence of DBs was shown in such 2D materials as graphene [19,20], on the edge of graphene nanoribbon [21-22], boron nitride [23], and in other carbon polymorphs [24, 25].

In the present work, clusters of DBs consisting of two and three closely placed DBs are studied by molecular dynamics simulation. Energy exchange between DBs is observed and discussed in relation to graphane dehydrogenation. Effect of temperature on the life time of DB is shown for 50 K for single DB in thermal equilibrium.

2. Simulation details

The initial configuration of graphene sheet is achieved by locating all the carbon atoms in a planar honeycomb lattice with the interatomic distance equal to 1.55 Å. The hydrogen atoms are bonded to the graphene sheet on both sides alternatively with the bond length 1.1 Å. Two types of boundary conditions are considered. The first type is periodic boundary conditions (PBC) applied along x and y directions to create infinite structure. For the second type, PBC are applied only along y direction, while atoms on the borders of the simulation cell along x axis are fixed. Initial structure can be found in the previous work on DBs in graphane [15], together with the full description of single DB in graphane.

The simulation is performed using the large-scale atomic/molecular massively parallel simulator (LAMMPS) package [26] with the adaptive intermolecular reactive empirical bond order (AIREBO) potential [27]. AIREBO interatomic potential can be used to model both chemical reactions and intermolecular interactions in condensed-phase hydrocarbon systems and was successfully used for the simulation of discrete breathers in graphane [15], investigation of thermal and mechanical properties in carbon nanostructures [28-31]. It is worth mentioning that the molecular dynamic (MD) approach could lead to significant errors for the investigations of breathers with large amplitudes. The reason is that the empirical potentials for the molecular dynamics calculations are constructed to describe mainly the linear properties (such as frequencies of phonon modes or elastic constants) of the correspondent physical system. Discrete breathers being essentially nonlinear objects should be treated with more adequate approximations to take into account such effects as the deformation of atom electron shells in the oscillation process. In this regard we refer to the paper [16], in which DBs have been investigated in graphane in the framework of the density functional theory (DFT) [32] that provides quantum-mechanical approach. It was shown that the striking difference of the DBs properties in the MD and DFT simulations emerges while the amplitude of the hydrogen atom

vibrations reaches the value of 0.15 \AA . The main difficulty of using the quantum-mechanical techniques is that they are very time consuming especially for the simulations of the atoms dynamics. Therefore for the investigation of energy exchange on long time intervals in DB clusters the molecular dynamics is still the most preferable approach.

In the study of DB clusters, initial temperature of the simulation cell is set to be zero. To reach the equilibrium state, the simulation cell is relaxed with the Nose-Hoover thermostat during 50 ps with the time step 0.5 fs. Since carbon atoms are slightly displaced by the hydrogen atoms out of the plane during relaxation, small deformation is applied to the simulation cell. This simulation is performed under the constant volume and energy ensemble. As a result, the graphane structure in further experiments is characterized by the distance between C atoms equals to 1.55 \AA and between C and H atoms equals to 1.1 \AA (which is in a good agreement with theoretically predicted values [33]).

Two types of DB clusters considered in this paper are shown in Fig. 1: clusters consisting of two (A-C) and three (D-F) DBs. For each case, three different types of initial atomic displacements in the clusters are applied as it is shown in Fig. 1. For the cases A-C, two DBs can be excited by displacing the atoms 1-2, 1-3 and 1-4. All the other two DBs combinations of atoms will be symmetrically similar to the ones mentioned above, because within the considered six-atom circle only named combinations can lead to the different scenarios. Arrows in Fig. 1 show the directions of initial atomic displacements and thus describe the initial conditions. The DB cluster is placed in the middle of the computational cell. During each simulation, the displacements and kinetic energy of DBs are recorded to study the energy exchange between DBs. For the clusters of three DBs, D-F, there are also three symmetrically different types of initial atomic displacements: atoms 1, 2 and 3, atoms 1, 2 and 4, and atoms 1, 3 and 5 are to be displaced. A more detailed discussion on the symmetrical properties of discrete breathers in 2D lattice can be found in [34].

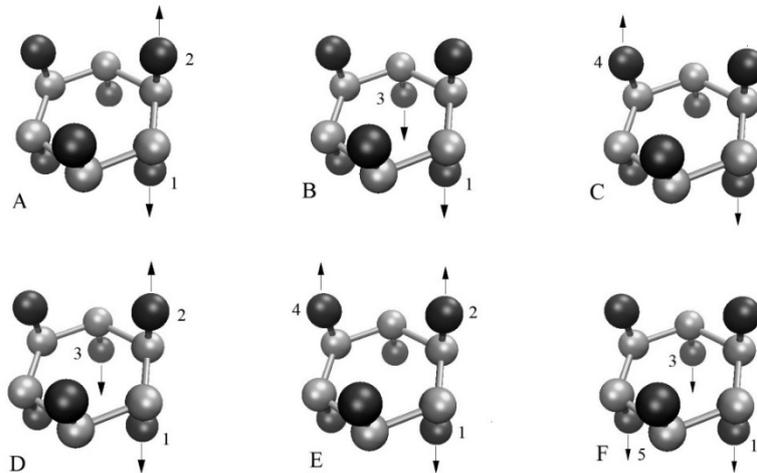


Fig. 1. DB clusters in graphane. Light balls depict carbon atoms and dark balls show hydrogen atoms. The possible directions of the initial atomic displacements are shown by arrows. Vibrating atoms in the clusters are numbered.

The effect of boundary conditions is studied for all the clusters. As the example, kinetic energy of atoms averaged over oscillation period in DB cluster D excited with initial displacements $u_1=u_3=-0.1 \text{ \AA}$, $u_2=0.08 \text{ \AA}$ is shown in Fig. 2 as the function of time. Curves for PBC along x and y directions are shown by solid lines and for PBC only along x direction are shown by dashed lines. As it can be seen, there is no qualitative difference in the energy flow. The main difference is in the period of the energy exchange between DBs. In the following,

only the results for PBC along both x and y directions are presented, but for some clusters the effect of PBC is mentioned in case of any qualitative deviations of the results.

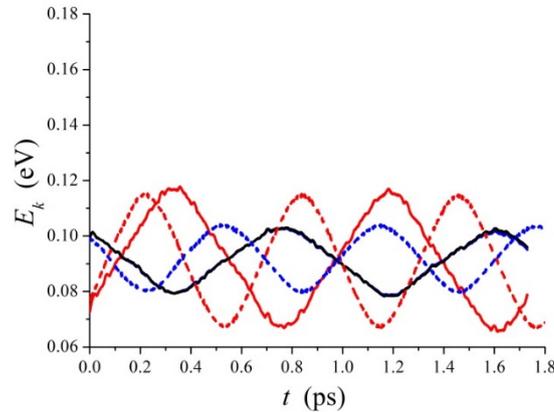


Fig. 2. Results for two types of boundary conditions for the DB cluster D excited with the initial atomic displacements $u_1=u_3=-0.1 \text{ \AA}$, $u_2=0.08 \text{ \AA}$. Solid lines are for PBC along x and y directions and dashed lines for PBC along x direction. Black line corresponds to the DB_1 , red line to the DB_2 and blue line to the DB_3 .

3. Results and Discussion

3.1. Clusters of discrete breathers. The main thing which should be considered for clusters of DBs is the effect of the difference in its initial amplitudes and phases. Both these parameters can cause different scenario for atomic movement and energy exchange between DBs in the clusters. In our experiments, the value u_i determinates the initial displacement of the H atom in the discrete breather with number i , while the sign of this displacement indicates the initial phase.

Kinetic energy of atoms in DB as the function of time is shown in Fig. 3 for clusters consisting of two breathers in the form A (a, b), C (c) and B (d-f). Different scenario of energy exchange can be found for different initial conditions. Two typical examples which can characterize the breathers behavior in cluster A are shown in Fig. 3 a, b. For all the cases of initial conditions including difference in the initial amplitudes and phases, the energy exchange between DBs is found. Interestingly, for cluster C, which is similar to cluster A because in these cases one hydrogen atom is above the graphene plane and second atom is below the graphene plane, no energy exchange is observed for positive initial phases. Slow energy exchange is found for negative phase (Fig. 3 c), both for different and equal amplitudes.

More complicated scenario can be observed for cluster B, where both hydrogen atoms are placed below the graphene sheet. Figure 3 d shows kinetic energy as the function of time for $u_1=u_3=-0.1 \text{ \AA}$ which is the same for $u_1=u_3=0.1 \text{ \AA}$. Difference in the initial displacements of hydrogen atoms leads to qualitatively different scenario of energy exchange. If for equal amplitudes energy exchange can be found just for small period of time, for different initial amplitudes it takes place during entire simulation run. For the last example (Fig. 3 f), when difference in the initial phase is introduced together with the difference in the initial amplitudes, slow energy exchange can be found.

For most cases, decrease of the DB amplitudes is found, while for some cases (see Fig. 3 b, c and f) the amplitude of one of DBs in the cluster does not decrease. It can be concluded, that even small difference in the initial conditions can lead to various scenarios and cause different energy exchange between DBs.

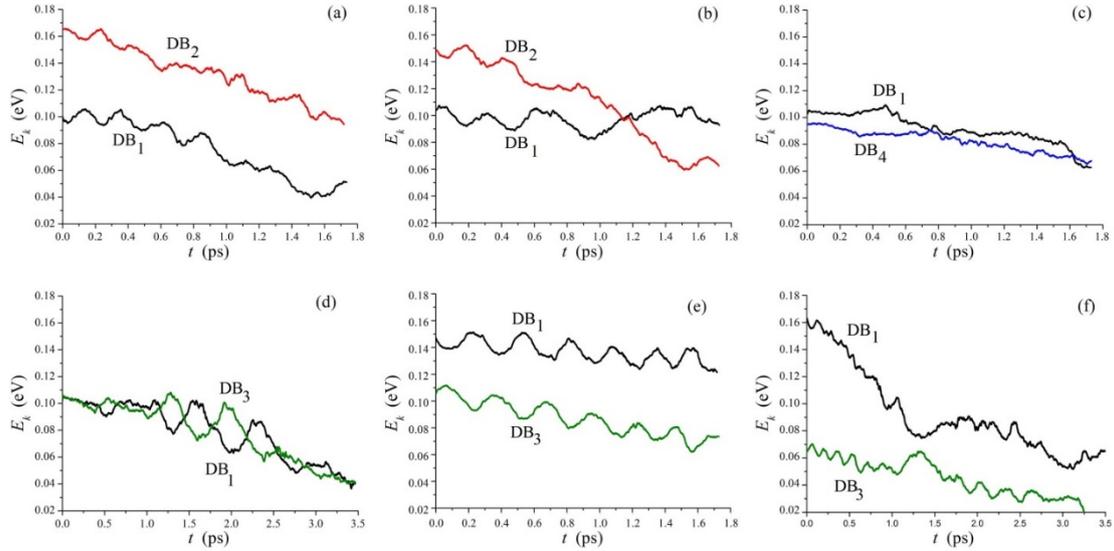


Fig. 3. Kinetic energy of DBs averaged over oscillation period as the function of time for (a) cluster A $u_1=u_2=0.1 \text{ \AA}$, (b) cluster A $u_1=-0.08 \text{ \AA}$ and $u_2=0.1 \text{ \AA}$, (c) cluster C $u_1=-0.1 \text{ \AA}$ and $u_4=-0.08 \text{ \AA}$, (d) cluster B $u_1=u_3=-0.1 \text{ \AA}$, (e) cluster B $u_1=0.1 \text{ \AA}$ and $u_3=0.08 \text{ \AA}$ and (f) cluster B $u_1=0.1 \text{ \AA}$ and $u_3=-0.08 \text{ \AA}$. Black curves are used for DB₁, red curves - for DB₂, green curves - for DB₃ and blue curves - for DB₄.

For cluster D, two cases of DBs interaction can be considered: (i) simultaneous excitation of DB₁ and DB₂ with the different initial conditions for DB₃ and (ii) simultaneous excitation of DB₁ and DB₃ with the different initial conditions for DB₂. Three various scenarios for each case are shown in Figs. 3 and 4. As it can be seen, for all the initial conditions energy exchange takes place, but in a different way. When the initial amplitude of all atoms are the same (Fig. 3, a) quite intensive energy exchange can be seen both for positive and negative initial phase of vibrations. In case, when the difference of the amplitudes is introduced, the increase of the kinetic energy of DB₃ takes place together with the decrease of the energy of DB₂. Simultaneously, DBs in the cluster exchange the energy between each other. The other scenario of energy exchange is found for the DBs excited with the different amplitudes and with negative initial displacement ($u_1=u_2=-0.1 \text{ \AA}$, $u_3=-0.08 \text{ \AA}$): there is an active energy exchange between DB₁ and DB₃, while DB₂ just slightly participates in this process. The similar behavior is found for initial conditions $u_1=u_2=0.1 \text{ \AA}$, $u_3=0.1 \text{ \AA}$ and $u_1=u_2=-0.1 \text{ \AA}$, $u_3=-0.1 \text{ \AA}$ (Fig. 3, a) and $u_1=u_2=0.1 \text{ \AA}$, $u_3=0.08 \text{ \AA}$ and $u_1=u_2=-0.1 \text{ \AA}$, $u_3=0.08 \text{ \AA}$ (Fig. 3, b).

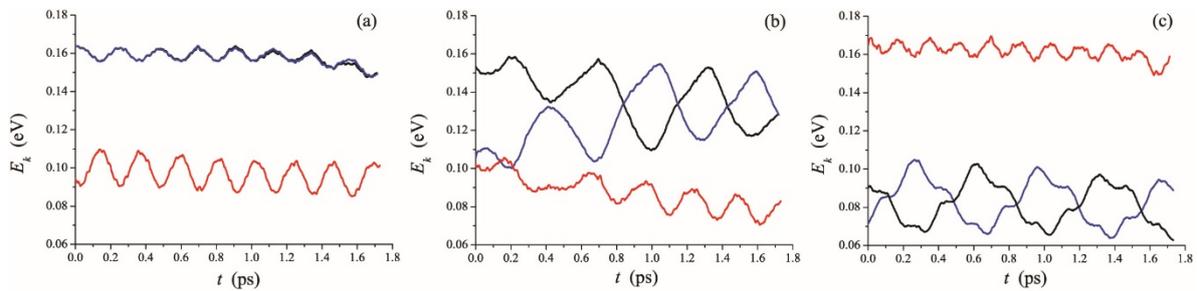


Fig. 4. Kinetic energy of DBs averaged over oscillation period as the function of time for cluster D for (a) $u_1=u_2=0.1 \text{ \AA}$, $u_3=0.1 \text{ \AA}$, (b) $u_1=u_2=0.1 \text{ \AA}$, $u_3=0.08 \text{ \AA}$ and (c) $u_1=u_2=-0.1 \text{ \AA}$, $u_3=-0.08 \text{ \AA}$. We use black line for DB₁, red line for DB₂ and blue line for DB₃.

The other three types of system behavior are found for simultaneous excitation of DB₁ and DB₃ with the different initial conditions for DB₂. This case is more symmetric than the first one, because DBs 1 and 3 are placed below the sheet and DB₂ is placed above it. Thus,

synchronous excitation of DBs under the sheet with DB₂ leads to significant difference in the results. Figure 4, a shows no energy exchange between DBs for initial conditions $u_1=u_3=-0.1 \text{ \AA}$, $u_2=0.1 \text{ \AA}$ and $u_1=u_3=0.1 \text{ \AA}$, $u_2=-0.1 \text{ \AA}$, which means that changes in the initial phases do not lead to the energy exchange if the amplitude is the same. Figure 4, b shows the slight energy exchange between DBs for $u_1=u_3=0.1 \text{ \AA}$, $u_2=0.08 \text{ \AA}$ and Fig. 4, c shows slow but considerable energy exchange between DB₂ and DBs 1 and 3. Figure 4, c is for $u_1=u_3=-0.1 \text{ \AA}$, $u_2=0.08 \text{ \AA}$ and $u_1=u_3=0.1 \text{ \AA}$, $u_2=-0.08 \text{ \AA}$. It can be concluded that the difference in the phases does not lead to the changes in the scenario of energy exchange, while difference in the initial amplitudes can lead to the considerable changes.

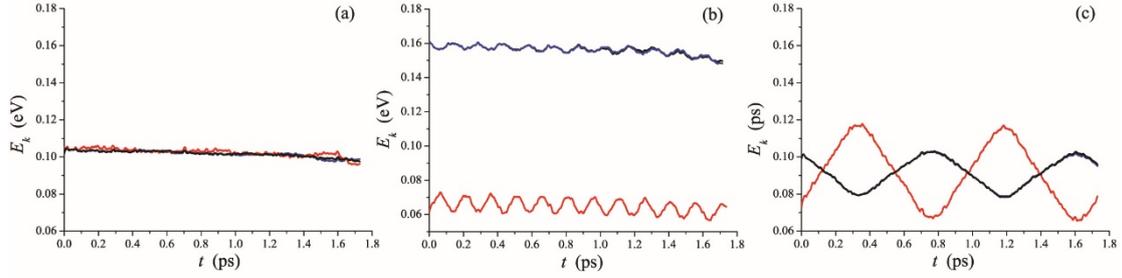


Fig. 5. Kinetic energy of DBs averaged over oscillation period as the function of time for cluster D for (a) $u_1=u_3=-0.1 \text{ \AA}$, $u_2=0.1 \text{ \AA}$, (b) $u_1=u_3=0.1 \text{ \AA}$, $u_2=0.08 \text{ \AA}$ and (c) $u_1=u_3=-0.1 \text{ \AA}$, $u_2=0.08 \text{ \AA}$. Black line is used for DB₁, red line for DB₂ and blue line for DB₃.

Figure 5 shows the averaged kinetic energy of DBs as the function of time for cluster E. Two combinations can be considered: DBs 2 and 4 are excited with the same displacements and DB₁ is excited with different displacement (more symmetric case) and DBs 1 and 4 are excited with the same displacements and DB₂ – with the other initial displacement. Similarly to cluster D, in more symmetric case for $u_2=u_4=-0.1 \text{ \AA}$, $u_1=0.1$ no energy exchange can be found (Fig. 5, b), while the difference in the initial amplitudes lead to the slight energy exchange which is not dependent on the difference in the initial phases. Example of energy exchange for initial conditions $u_1=u_4=-0.1 \text{ \AA}$, $u_2=-0.08 \text{ \AA}$ is shown in Fig. 5, b and represents DBs behavior for $u_1=u_4=-0.1 \text{ \AA}$, $u_2=0.08 \text{ \AA}$, $u_1=u_4=0.1 \text{ \AA}$, $u_2=0.08 \text{ \AA}$, which means that difference in the initial amplitudes and phases cannot lead to the considerable changes in the energy exchange. The same is for the case DB_{2,4} and DB₁. Figure 5, a represents DBs behavior for $u_2=u_4=0.1 \text{ \AA}$, $u_1=0.08 \text{ \AA}$ and $u_2=u_4=-0.1 \text{ \AA}$, $u_1=0.08 \text{ \AA}$.

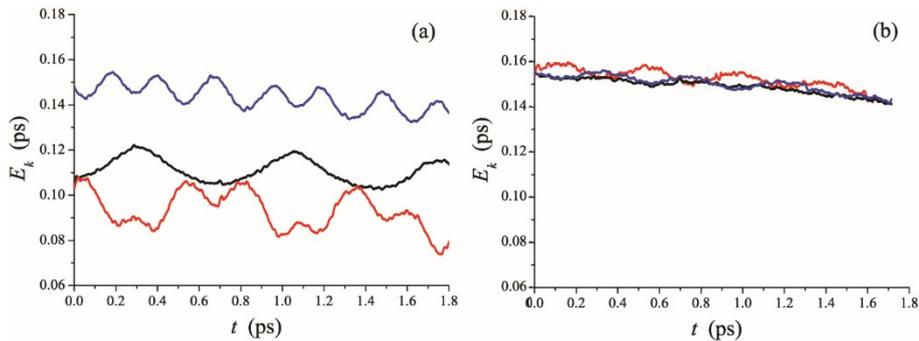


Fig. 6. Kinetic energy of DBs averaged over oscillation period as the function of time for cluster E for (a) $u_1=u_4=-0.1 \text{ \AA}$, $u_2=-0.08 \text{ \AA}$ and (b) $u_2=u_4=-0.1 \text{ \AA}$, $u_1=0.1 \text{ \AA}$. Black line stands for DB₁, red line for DB₂ and blue line for DB₃.

In Fig. 6, kinetic energy of DBs averaged over oscillation period, E_k , for cluster F is shown as the function of simulation time for two types of initial conditions: (a) $u_1=u_3=0.1 \text{ \AA}$, $u_5=-0.1 \text{ \AA}$ and (b) $u_1=u_3=0.08 \text{ \AA}$, $u_5=-0.1 \text{ \AA}$. As it can be seen, two DBs initially excited with

the same amplitude $u_1=u_3=0.1 \text{ \AA}$ move together during all the simulation time in both cases. The main difference between these two figures is that (a) shows the effect of phase difference and figure (b) shows the effect of difference in the initial amplitude. In the case, when DBs 1 and 3 are excited with the same phase as DB₅ the energy exchange can be seen both for $u_1=u_3=u_5$ and for $u_1=u_3=0.8u_5$, which is shown in Fig. 7 (a). From Fig. 7 (b) a considerable energy exchange with a low period between breathers 1 and 3 and DB₅ can be seen.

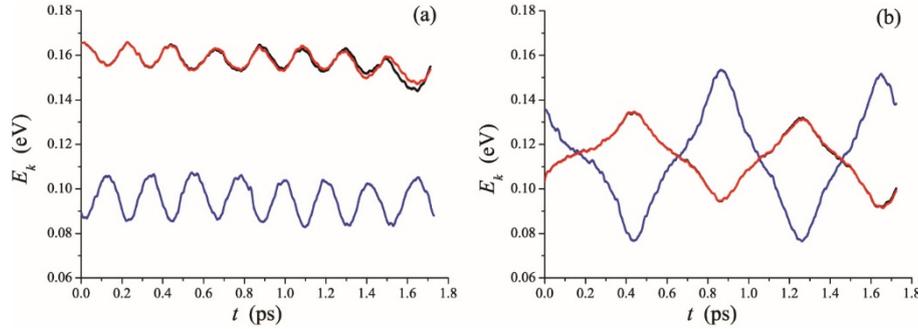


Fig. 7. Averaged kinetic energy of DBs as the function of time for cluster F for (a) $u_1=u_3=0.1 \text{ \AA}$, $u_5=-0.1 \text{ \AA}$ and (b) $u_1=u_3=0.08 \text{ \AA}$, $u_5=-0.1 \text{ \AA}$. Black line is for DB₁, red line - for DB₃ and blue line - for DB₅.

3.2. Discrete breathers in thermal equilibrium. DBs in thermal equilibrium are studied at temperature 50 K. Quite low temperature was chosen from consideration that at low temperatures life time of DBs would be much longer than at high temperatures. Nose-Hoover thermostat is used for system thermalization during 5000 simulation steps after which DB is excited. Simulation at finite temperatures are conducted to find the time until DB is dying averaged over at least 100 trials at given conditions.

In Fig. 8, kinetic energy of DB (black curve) in comparison with the average kinetic energy of the system (gray curve) are shown as the functions of simulation time. As it can be seen, energy of DB gradually decreases to the average value of the system kinetic energy. Fig. 8 presents one example of DB life in thermal equilibrium, where the average life time is about 7 ps. The life time of DB is defines as the time when kinetic energy of DB become close to the average kinetic energy of the crystal.

After averaging over 100 realizations, the live time of DB is found to be 9 ps. It means that DBs in graphane can live in thermal equilibrium during quite a long time.

4. Conclusions

Clusters of DBs and energy exchange between DBs in clusters are studied by molecular dynamics simulation at zero temperatures in graphane. In general one can conclude that behavior of studied earlier separate DBs in graphane [16,35] and DB clusters is similar. Another feature of soft nonlinearity high localized DBs in graphane by comparison to DBs in graphane [20-21] is the extended lifetime. However, in graphane a possible contribution of DB to mechanical behavior of the material in case of considering it as a mechanical continuum [36-38] can be more noticeable.

Various initial conditions for excitation of cluster consisting of two and three DBs are considered. Results for two types of boundary conditions are compared. No qualitative differences are found for both types of the boundary conditions and most of the reported results are for periodic boundary conditions applied in both x and y directions.

It is shown that clusters of DBs stay stable for a long time for all considered initial conditions. More important is that some initial conditions lead to considerable energy exchange between breathers in clusters. Both differences in the initial amplitudes and initial oscillation

phase of DBs significantly affect behavior of the clusters. As it is shown, difference in the initial amplitude of DBs in cluster is the main factor for energy exchange in the system.

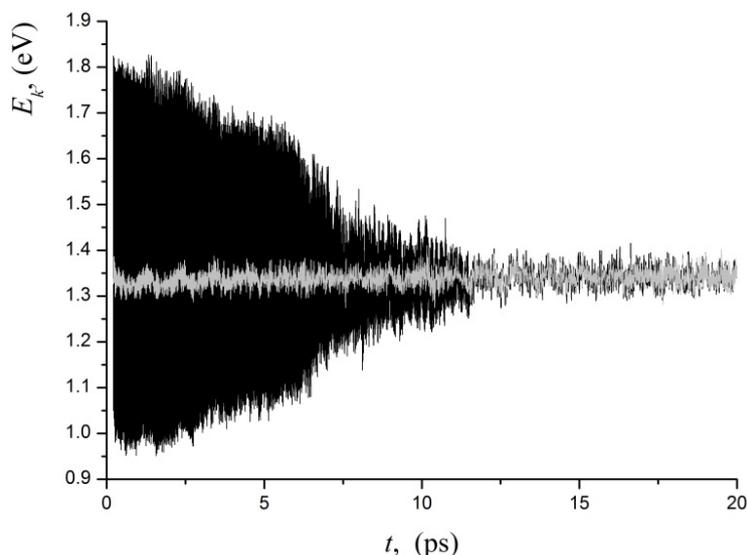


Fig. 8. Kinetic energy of DB (black line) and average kinetic energy of the system (gray line) as the functions of simulation time.

Studying of DBs in hydrogenated graphene (i.e., in graphane) is of high importance nowadays because DBs can be considered as the activators of dehydrogenation. This is so because DBs and their clusters are able to localize energy which is much higher than average kinetic energy of the system. Moreover, energy exchange between DBs in a cluster, or even irreversible energy transfer from one DB to another, lead to even higher energy localization and thus increase the probability of overcoming the dehydrogenation potential barrier for highly excited hydrogen atoms. Results presented in this work shed the light on the role of DBs in dehydrogenation of graphane at elevated temperatures [35].

The other decisive factor in hydrogenation/dehydrogenation process is temperature effect. In present work, only temperature equal to 50 K is considered for single DB in thermal equilibrium. It is shown for the first time that DBs in graphane can survive not only at zero temperature but also at finite temperature. However, the effect of temperature on the characteristics of DB should be considered further.

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