



Long-lived discrete breathers in free-standing graphene



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ABSTRACT

Intrinsic localized modes or discrete breathers (DBs) are investigated by molecular dynamics simulations in free-standing graphene. DBs are generated either through thermal quenching of the graphene lattice or by proper initialization, with frequencies and lifetimes sensitively depending on the interatomic potential describing the carbon-carbon interaction. In the most realistic scenario, for which temperature-dependent molecular dynamics simulations in three dimensions using a graphene-specific interatomic potential are performed, the DBs lifetimes increase to hundreds of picoseconds even at relatively high temperatures. These lifetimes are much higher than those anticipated from earlier calculations, and may enable direct breather observation in Raman spectroscopy experiments. Our simulations provide clear estimation for the temperatures in which DBs are expected to be thermally excited (1500–2000 K) representing a step forward for understanding the nonlinear physics of graphene and designing experiments in order to detect DBs, with possible impact in graphene-based future technological applications.

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1. Introduction

Recent technological achievements have allowed for the isolation of single graphene sheets either by chemical exfoliation of bulk graphite [1,2] or by epitaxial growth on metal substrates through thermal decomposition of SiC [3]. As a truly two-dimensional (2D) system, it provides a framework for new type of electronic and magnetic devices [4]. While the electronic properties of graphene have been exhaustively investigated [5], its mechanical and thermal properties are not quite thoroughly analyzed. In particular, while a reliable linear phonon spectrum can be obtained numerically and compared with the experimental one, much less is known about the nonlinear vibrational modes in graphene. Since all potentials used for modelling the vibrational properties of graphene are nonlinear, it is natural to expect that intrinsic localized modes, i.e. discrete breathers (DBs), may be formed. DBs are spatially localized and time-periodic vibrational modes that form spontaneously in nonlinear lattices [6–8]; they have been assessed experimentally in several systems, including solid state mixed-valence transition metal complexes [9], quasi-one dimensional antiferromagnetic chains [10], micromechanical oscil-

lators [11], optical waveguide systems [12], Josephson-junction arrays [13,14], proteins [15], and NaI crystals [16].

DBs have been studied in graphene using MD in graphene [17,18], strained graphene [19–21], graphene [22] and in carbon nanotubes [23,24]. Recently they have been studied as well using *ab initio* MD techniques in graphene [25] and graphene [26].

A reliable computational prediction of possible DB excitations in graphene, their lifetime and spectral features, will enable their direct experimental observation and facilitate the design of efficient future devices at relatively high temperatures. In the present work we perform extensive molecular dynamics (MD) simulations that reveal the existence of DBs in free-standing graphene both at zero temperature in 2D as well as at finite-temperatures in three dimensions (3D). To this end, we resort to Sandia National Laboratories Large-Scale Atomistic/Molecular Massively Parallel Simulator (LAMMPS) [27]. In order to demonstrate the DB onset and stability range we have tested several interatomic potentials (IPs) that have been utilized in the past to model carbon systems (Tersoff [28], AIREBO [29], LCBOP [30], CBOP [31], among others). However, we eventually focus on a graphene-specific Tersoff potential [28], hereafter referred to as Tersoff10, which is of the form

$$E_{ij} = V_{ij}^R + b_{ij}V_{ij}^A \quad (1)$$

The functions $V_R(r)$ and $V_A(r)$ are pair-additive interactions that represent all interatomic repulsions (core–core, etc.) and attraction

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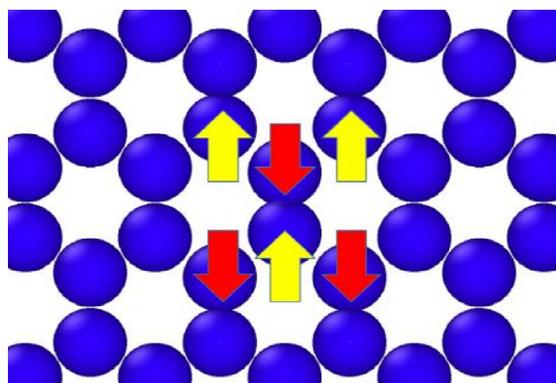


Fig. 1. Schematic illustration of the initial condition to generate discrete breathers (arrows are not at scale).

from valence electrons, respectively. The quantity r_{ij} is the distance between pairs of nearest-neighboring atoms i and j and b_{ij} is a bond order between atoms i and j . As it would be expected, the stability and lifetimes of DBs in graphene is strongly potential-dependent [17–21]. AIREBO and LCBO potentials include angular, dihedral (out of plane distortions), as well as long-range terms. The comparison of the results obtained using AIREBO and LCBO points to a destructive effect of the long-range part of the potentials on the stability of the DBs. This is more evident when LCBO is compared with the CBOP. The Tersoff10 potential is a reparametrized version of the original Tersoff89 IP that provides much better agreement with the experimental phonon velocities and frequencies, without significantly altering the agreement to other structural data. The choice of that potential is based on its performance on particular features regarding the vibrational properties of graphene. Along with LCBO, the Tersoff10 IP provides the most accurate overall description for its phonon dispersion curves. In particular, the Tersoff10 IP produces more accurate LA and ZA branches but less accurate ZO and TA branches than LCBO at temperature $T = 300$ K. Moreover, it is the only one to produce a linear temperature-dependence of the doubly degenerate Raman active E_{2g} mode of the Γ point [32]. We consider these two features important for the correct simulation of DBs in free-standing graphene.

The temperature-dependence of the vibrational graphene spectra was investigated using the original Tersoff89, Tersoff10, LCBO, and AIREBO potentials. The MD simulations were performed using a periodic triclinic computational cell of 20×20 unit cells (overall 800 carbon atoms). The computational cell was relaxed for each potential and the corresponding lattice parameter was calculated and used in defining the BZ edges in each case. A very

fine time-step of 0.05 fs was used and the trajectory and velocities were saved every 10 time-steps. These simulations typically run for about 32.8 ps each (655,360 time-steps). For the Tersoff10 potential, the graphene vibrational response was analyzed by producing the dispersion curves at temperatures $T = 60$ K, 500 K, and 1500 K [30]. For that IP, the strongest temperature-dependence is observed on the optical branches. Upon increasing of temperature, the frequencies lower by as much as 64 cm^{-1} (~ 2 THz).

2. Results

2.1. NVE simulations

Discrete breathers in graphene may be generated by either local initial displacements (and subsequent MD evolution), or by thermal quenching of the graphene lattice. The former method consists of displacing a few atoms deeply in the graphene lattice according to an approximate solution obtained by the rotating wave approximation of the equations of motion (Fig. 1) [33]. The simulations were carried out in the microcanonical ensemble (NVE) in 2D using the Tersoff10 potential with a time-step $\Delta t = 10^{-5}$ ps and periodic boundary conditions. The graphene samples typically contain 15,000 atoms, so that edge effects do not affect DB stability.

Finite size effects have been investigated by performing repeated simulations using computational cells of different sizes. The initial displacement, d , ranges from 0.1 to 0.3 \AA (We limited ourselves to displacements just up to 0.3 \AA since larger displacements can create defects, even trigger melting, instead of generating stable DBs). Depending on the value of d , two different DB configurations, say Type-1 and Type-2, have been observed. Type-1 breathers are observed for d in the range $0.15\text{--}0.19 \text{ \AA}$ (Fig. 2a), while type-2 DBs are observed for d in the range $0.27\text{--}0.3 \text{ \AA}$ (Fig. 2b). Both Type-1 and Type-2 DBs exhibit almost steady evolution for relatively long times. The *central* atoms of Type-1 DBs (red atoms in Fig. 2a) execute large amplitude periodic oscillations while the outer ones (blue atoms in Fig. 2a) small amplitude oscillations. Typical oscillation patterns of the inner (central) and outer atoms of a Type-1 DB are shown in Fig. 3 (supporting information video 1). The phases of large and small amplitude oscillations differ by π in that DB configuration. The frequency of the oscillations of the inner atoms here is not constant with time but increases up to twice its value at the same time that the amplitude of the oscillations clearly decreases (after 20 ps). The periodicity is not exact so these DBs could be seen as well as quasi-breathers, as in the work of Chechin et al. [34].

The configuration of Type-2 DBs is much more complex and only some of the atoms exhibit regular oscillations (supporting information video 2). In both types of DBs however the energy remains almost constant for long times, during which their fre-

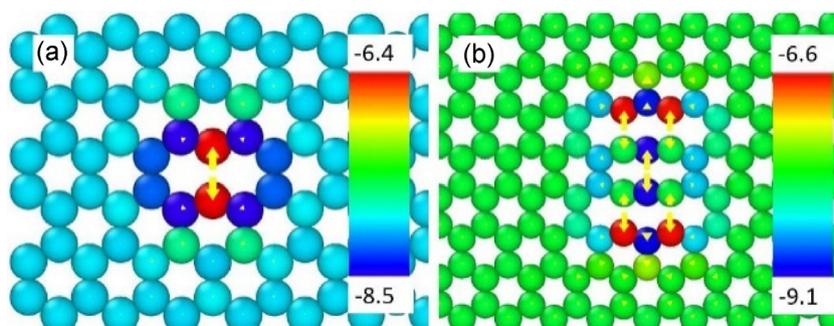


Fig. 2. Type-1 (a) and Type-2 (b) breathers in a single graphene sheet at $T = 10$ K. Color scale correspond to the total energy in eV/atom. The yellow arrows show the displacements with respect to the equilibrium position after stabilization. The length of the arrows is 3 times the real value for the shake of clarity. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

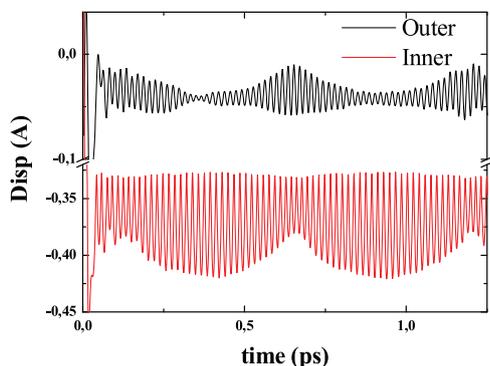


Fig. 3. Displacement in the y direction (in Å) of inner (red line) and outer (black line) atoms in a Type-1 breather. Notice the break in the y -axis. Both oscillations correspond to a frequency ~ 56 THz. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

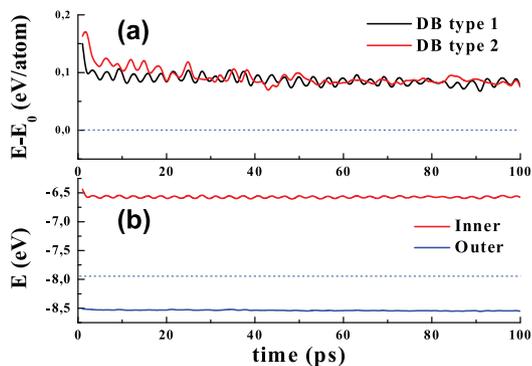


Fig. 4. a) Time evolution of the total energy per atom, of the two types of DBs, minus the background energy E_0 (blue dashed line), in eV/atom. b) Time evolution of the total energy of the inner and outer atoms in a type-1 DB compared to the background energy (blue dashed line). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

Table 1

Properties of Type-1 and Type-2 DBs observed in NVE simulations in 2D using the Tersoff10 potential, where d is the initial displacement, ν and A the frequency and amplitude of the oscillations, respectively, τ the calculated lifetime, and E_{ex} the excess energy stored in the DB.

DB type	Properties				
	d (Å)	ν (THz)	A (Å)	E_{ex} (eV/at)	τ (ps)
1	0.15–0.19	56 ± 0.4	0.11	0.1	500 ± 50
2*	0.27–0.31	59 ± 1	0.05	0.1	450 ± 50

* The oscillation corresponds to the outer atoms in dark blue (Fig. 2b).

frequency is calculated to be ~ 56 THz, i.e., above the highest frequency of the upper optical phonon dispersion branch. In Fig. 4a, we show the average value of the energy of DBs type-1 and 2 considering 6 and 8 atoms respectively (red and dark blue atoms in Fig. 2) minus the energy in equilibrium, E_0 , what gives a similar value in both cases and a similar slow decay with time. If we consider only the two inner atoms in the type-1 DB (like in ref [17]) then the energy of the breather is about 2.8 eV (See Fig. 4b). From an extrapolation of the energy decay, we can estimate the lifetime of Type-1 and Type-2 DBs to be 500 ps and 450 ps, respectively. The properties of Type-1 and Type-2 DBs obtained from the NVE simulations in 2D using the Tersoff10 potential are summarized in Table 1. The original Tersoff potential is soft (the frequency of localized modes reduces with increase in amplitude, while the opposite stands for a hard potential) and no DBs are stable. On the contrary, the 2010 version is a hard potential and long-lived DBs are clearly found. The calculated DB lifetimes using

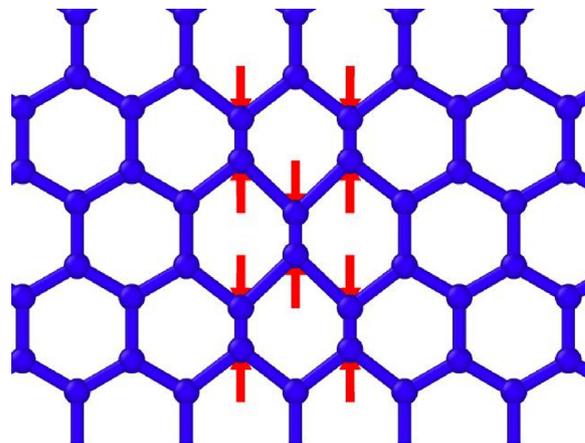


Fig. 5. Schematic illustration of an alternative initial condition to generate Type-2 discrete breathers (arrows are not at scale).

the Tersoff10 potential are much longer than those reported before, e.g., in finite-temperature simulations using the Brenner potential (~ 1 ps at $T = 10$ K) [17] and in MD simulations using an AIREBO-type potential (~ 30 ps) in strained graphene [19]. The corresponding breather frequencies have been reported to be 47 THz and ~ 27 –32 THz, respectively.

Interestingly, type-2 breathers can be regarded as a cluster of five type-1 DBs put together, two above and two below the central one. This is not just an assumption looking at the geometry of the type-2 DB. Indeed, the type-2 breather can also be created by moving 10 atoms (initial displacement ranging from 0.15 to 0.26 Å) as shown in Fig. 5. It has to be mentioned that clusters of breathers have been studied recently in the work of Baimova et al. [20]. Type-2 DB is effectively a cluster of 5 DBs as shown in Fig. 1c. E of ref. [18]

2.2. Temperature effect

We now turn our attention to the effect of temperature on the stability of the DBs. The graphene sample is first equilibrated to the desired temperature for 10 ps. A DB is then created by applying suitable initial displacements, as described earlier, and the simulation continues keeping the temperature constant at the desired value. It is anticipated that the DB lifetime is temperature-dependent since thermal noise will eventually destroy its stability. The results presented so far were constrained in 2D for simplicity; that constraint, however, excludes the possibility of off-plane phenomena by completely quenching intrinsic thermal rippling [35–37]. For that reason, our finite-temperature NPT simulations at zero pressure are performed in 3D and reveal that both Type-1 and Type-2 DBs remain stable up to temperatures as high as 2000 K. Note that this is very near the melting temperature of graphene for the Tersoff10 potential, that is ~ 2100 K. The difference between the highest and lowest atomic displacements along the z -axis (perpendicular to the graphene plane) in a computational cell consisting of 15,000 atoms at high temperatures (from 1500 to 2000 K), resulting from the NPT simulations in 3D, is almost constant and around 15 ± 2 Å for a cell length of 250 Å. That curvature is rather small and moreover it is in good agreement with the experimentally obtained ones [38]. For temperatures increasing from $T = 300$ K to 2000 K, the curvature / corrugation increases but the DBs remain quite unaffected as far as their lifetime τ is concerned (supporting information video 3). For small initial displacements of the order of 0.1 Å, the DBs are very sensitive to thermal vibrations; even at temperatures as low as 10 K, they can be easily destroyed. For larger displacements, the DBs are

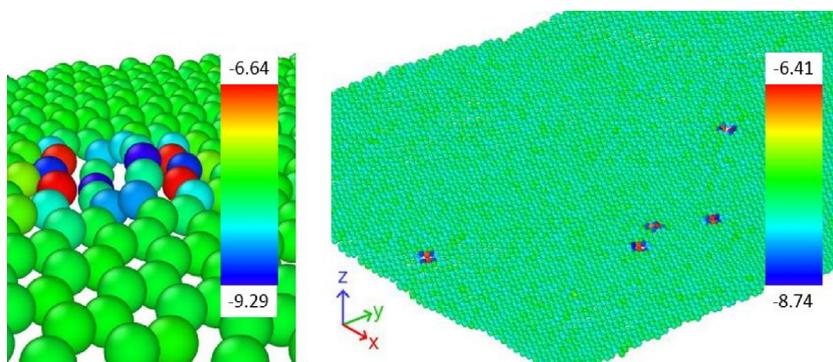


Fig. 6. (a) Type-2 DB in a graphene sheet heated at 1700 K in 3D. The breather structure is tilted out of plane; (b) Type-1 breathers in a graphene sheet after quenching from 1600 K. The rainbow scales represent the total energy in eV/atom.

Table 2

Breather lifetimes at high temperatures as a function of the initial displacement. When the temperature is lower than T_C the lifetime is at least the one quoted in the second row. For all displacements but $d=0.3$ Å the DBs are of Type-1, while for $d=0.3$ Å the breathers are of Type-2.

Disp (Å)	0.1	0.15	0.2	0.25	0.3
T_C (K)	10	500	1900	2000	2000
Lifetime (ps)	< 0.5ps	> 500	> 500	> 500	> 500

stabilized despite high temperatures, with recorded lifetimes longer than $\tau \sim 500$ ps. For example, if the displacement is 0.15 Å (0.2 Å), the Type-1 DB remains stable for long times if the temperature is lower than a critical one, $T_C = 500$ K ($T_C = 1900$ K). At high temperatures ($T > 1500$ K), the DB structure is slightly distorted as compared to the symmetric configurations in Fig. 2. However, some atoms still remain in a higher or a lower energy level for long times (more than 500 ps). The DBs created with initial displacements 0.25 (of Type-1) or 0.3 Å (of Type-2) can be regarded to be stable even at $T = 2000$ K. A typical Type-2 DB configuration is shown in Fig. 5a with its 3D structure being tilted out of plane. Table 2 summarizes the results of this paragraph.

The value of the critical temperature T_C clearly depends on the initial displacement used to generate a DB, as well as the type of the DB; for $T > T_C$, however, both types of DBs rapidly decay. Generally speaking, the T_C of a particular DB increases with increasing the initial displacement, d , indicating that more energetic breathers survive for longer times. Importantly, at $T > 1600$ K, thermal excitation of DBs has been observed (supporting information video 4). Notably, thermal excitation of DBs that arise from anharmonicity, that is expected to be strong at high temperatures, has been also demonstrated in ionic perfect crystals [39].

Temperature effects upon DB lifetimes can be better understood by analysing the corresponding effects on the phonon dispersion curves. The frequency of the LO/TO modes slightly decreases with increasing temperature with a rate very closed to that experimentally observed [40]. At the same time, the DB oscillation frequency (of Type-1 here), or more precisely the oscillation of the inner (central) atoms shown in red colour in Fig. 2a, decreases faster and drops below that of the LO/TO modes at temperatures higher than 400 K. At such temperatures, the interaction with the (linear) LO/TO phonon modes removes energy from the DB which slowly decays (within a few hundreds of ps).

2.3. Thermal quenching

A better suited for experiments and perhaps more natural method for DB generation is that of thermal quenching [41,42].

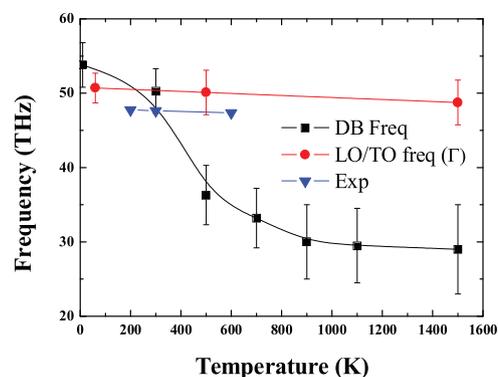


Fig. 7. Type-1 breather frequency (black squares) and LO/TO frequency modes at Γ point (red circles) for different temperatures. Experimental values from [35]. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

First, a graphene sample is heated up to a particular high temperature T_h above the Debye temperature in which all the phonon modes are populated. At that temperature, typically at $T_h > 1600$ K (in references [43,44] the values 2100 K and 2300 K are quoted, in reasonable agreement), the system is equilibrated for t_{eq} ps in the NPT (isothermal– isobaric) ensemble, and subsequently it is cooled down rapidly (quenching) to a relatively low temperature T_f . In our simulations, T_f ranges from 100 K to 500 K, while the effective quenching time is about 1–2 ps that correspond to quenching rates from 2000 K/ps to 1000 K/ps. In accordance with our results on the temperature-dependent lifetime of DBs, the number of DBs generated by thermal quenching does not depend significantly on the final temperature T_f as long as this is around room temperature.

However, the number of DBs at T_f does depend on the temperature T_h as well as the equilibration time t_{eq} at that temperature. Indeed, the number of DBs at T_f increases linearly with the equilibration time t_{eq} at T_h , while it increases exponentially with T_h . This is better seen in Fig. 8. Clearly the density of thermally created DBs increases linearly with the time t_{eq} . Also important, when the simulation is carried out in 3D the observed number of DBs created this way is more than twice (See inset in Fig. 8). The maximum density of DBs obtained by quenching the samples from 2000 K is about 2–4 per thousand atoms, distributed randomly in the sample (Fig. 6b). The interaction between DBs is weak, and each of them keeps its identity even though they may approach each other at distances less than 10 Å.

The density of DBs thermally created is negligible at low temperatures but, as we have seen, the DBs can survive for long time after quenching. The presence of these DBs can have a measurable

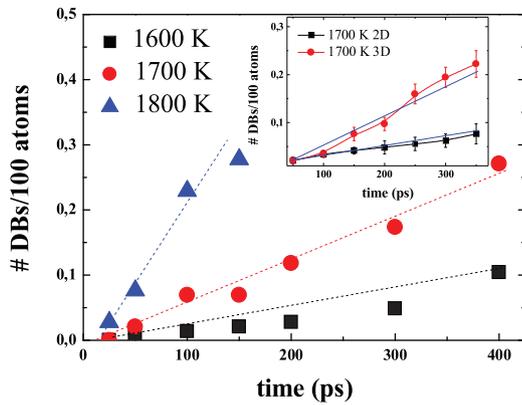


Fig. 8. Expected DBs density for different equilibration times at different temperatures as labelled. Inset shows the difference between 2D (black squares) and 3D simulations (red circles). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

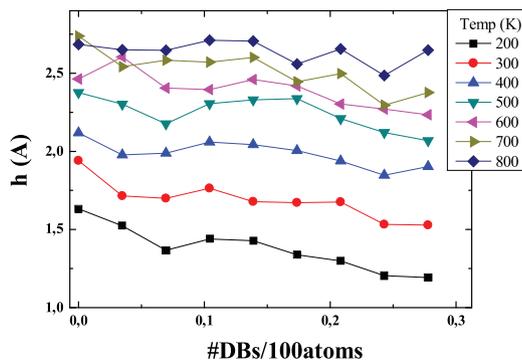


Fig. 9. Mean amplitude of the out-of-plane thermal fluctuation, h (in Å), vs the density of DBs for different temperatures as labelled.

effect in other properties of graphene like wrinkling and roughness for temperatures around room temperature. For example the mean amplitude of the out-of-plane thermal fluctuation, h , clearly decreases when the density of breathers increases, (See Fig. 9). Here h is calculated by a time averaged RMS (for 5 ps), namely

$$h = \sqrt{\sum_{i=1}^N \left\langle \frac{w_i^2}{N} \right\rangle} \quad (2)$$

where w_i is the out-of-plane displacement of the i th atom and N the total number of atoms. First a given density of breathers was randomly distributed in the graphene sheet using the method explained in section A, and then the sample was heated up to a certain temperature where the system is equilibrated for 50 ps. Fig. 9 shows the dependence of h with the density of DBs for different temperatures ranging from 200 K to 800 K.

As can be seen the effect is more evident at low temperatures (from 200 K to 500 K) while at higher temperatures the studied densities of DBs are not able to play a significant role in the wrinkling behaviour. Since there is a clear effect of the DBs and the way the layer of graphene bends and corrugates some interaction between the DBs and the acoustic modes could take place.

Another possible effect of some importance that the existence of DBs may have on the physical properties of graphene is a decrease in the thermal conductivity as the number of breathers increases. Breathers can be regarded as local distortions of the crystal lattice (or defects without cavities). Recently several papers have addressed the question of how different defects affect thermal [45,46] and elastic properties [47] of graphene. For example, Mehdi et al, showed that the introduction of small quantities (1%)

(of doping) nitrogen atoms in graphene's structure results in a considerable decline of the thermal conductivity of graphene by almost half of that of the ideal sheet [46].

3. Conclusion

In summary, the existence of long-lived DBs in a single graphene layer is demonstrated by MD simulations using the graphene-specific potential Tersoff10. The latter describes accurately the phonon dispersion curves, especially the optical branches, as well as their temperature-dependence. Moreover, it reproduces the linear temperature-dependence of the doubly degenerate Raman active E_{2g} mode of the Γ point [30]. These features make the Tersoff10 the most appropriate for the search of DBs in graphene and the reliable determination of their lifetimes and oscillation frequencies. Classical MD does not take into account quantum effects as electron-hole, mechanism that leads to a decay of the Γ point optical phonon on the time scale of 1 ps [48], or electron-electron interactions (e-e). However the frequencies of the DBs are well above the optical branch and thus the e-h interaction is not expected to be the dominant decay mode for a vibrational breather and the energies of the atoms forming the DBs are high compared to those far away, so the quantum treatment may be not necessary. More so, e-phonon (and also e-e) coupling could very well play a favorable role in the stability of the breathers as shown for simple systems by Wang et al. [49]. At any rate, experiments are necessary to check if our approach is correct or quantum corrections are important in this case.

DBs have been studied as well using other well-known interatomic potentials, as Tersoff, LCBO, CBOP and AIREBO. However, long-lived robust DBs were found only when using the newest version [28] of Tersoff potential (old Tersoff [50] (Tersoff88) and, for example, a somewhere more recent version [51] (Tersoff95) didn't produce stable DBs). As shown in previous works [17–21] the stability of the DBs is very sensitive to the details of the IP. When comparing LCBO with CBOP (which is very similar to LCBO but without long range terms) we found that the DBs are much more stable when using CBOP (the lifetime is, at least, 10 ps). However, the interaction range is not the determining factor since for the Tersoff88 and Tersoff95 IPs which have a similar range as CBOP, the DBs were not found to be stable.

We note that DBs can be created by different ways (initial conditions) that also affects the stability of the DB. For example, using AIREBO we found that moving just to atoms towards each other (only the two atoms in the central part of the DB, without moving the four atoms around like shown in Fig. 1) a DB is created that has a relatively long life (~ 10 ps) compared to that one observed moving the six atoms.

Finally our work does not merely provide additional evidence that DBs are likely to exist in graphene, but it makes lifetime predictions of the order of hundreds of picoseconds, much longer than those reported so far. Moreover, these lifetimes of graphene breathers persist when dimensionality increases from 2D to 3D. In 3D, the type-2 DBs abandon the symmetric configurations observed in 2D, and they acquire a 3D structure that is tilted with respect to the graphene plane. The distorted 3D breathers are fairly stable with hundreds of picoseconds lifetimes at high temperatures even close to the melting point. A non-negligible density of DBs have been also obtained by thermal quenching in NPT simulations in 3D at zero pressure. In this case we only obtain Type-1 breathers, implying that the thermal energy is not enough to excite Type-2 DBs. Higher temperatures result in a proliferation of defects and eventual melting. Our simulations provide a clear estimation for the range of temperatures in which DBs are expected to be thermally excited (above 1500 K and below 2000 K), as well as the dependencies of their number density. The present work

represents a step forward for understanding the nonlinear physics of graphene and designing experiments in order to detect DBs with possible impact in graphene-based future technological applications.

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Appendix A. Supplementary materials

Supplementary materials associated with this article can be found in the online version at <http://dx.doi.org/10.1016/j.chaos.2016.04.015>.

Video 1: Creation of a DB in a NVE 2D simulation. The initial displacement is 0.15 Å. Total simulation time 50 ps. Video 2: Creation of a DB in a NVE 2D simulation. The initial displacement is 0.3 Å. Total simulation time 50 ps. Video 3: The video shows how DBs are relatively unaffected in a NPT simulation. The graphene sheet is equilibrated at 100K and then some DBs are created as explained in Fig. 1. Then the sample is heated up to 1000K in a 500 ps ramp. Video 4: Example of a quenching simulation. The graphene sheet is heated up to 1600 K, equilibrated during 300 ps and then quenched to 300 K. Some randomly distributed DBs appear when the sample reaches some high temperature (and clearly remain when quenched).

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