Compact dislocation clusters in a two-dimensional highly ordered complex plasma

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Abstract. The mechanism and physics of defect nucleation are key questions that often remain open irrespective of the suggested melting scenario or the shear instability mechanism. Complex plasmas can serve as a powerful tool, providing a fundamental insight into the nucleation process generically. Either deformation-induced or thermally initialized nucleation in hexagonal plasma crystals starts with the appearance of compact dislocation clusters having a tetragon in the core. Hence, the competition for the minimal energy configuration between (stable) hexagonal symmetry and (unstable) tetragonal symmetry can be resolved in favor of a (meta-stable) ‘mixed symmetry’—a cluster of coupled dislocations in a hexagonal environment. Performing simulations with a specially designed tool—a deformable simulation cell—the mechanism of nucleation in two-dimensional plasma crystals is studied. The nontrivial topology of the dislocation clusters is explored in detail, and the results obtained agree well with experimental observations.

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1. Introduction

It is common knowledge that symmetry effects are crucial in three-dimensional (3D) and 2D systems. Different symmetries coexisting in the same phase and symmetry transformations escorting phase transitions are widespread in nature. For instance, the mechanisms of symmetry breaking are thought to be inherent in the molecular basis of life [1]. Chiral (mirror-isomeric) 2D clusters [2], magic clusters of a new symmetry ‘frozen-in’ by a solid surface [3], or dynamical symmetry breaking by the surface stress anisotropy of a two-phase monolayer on an elastic substrate [4] are examples of the importance of 2D or quasi-2D systems for many applications.

In this paper we address dynamical processes in highly ordered 2D complex plasmas associated with symmetry breaking accompanying nucleation, i.e. the creation of the dislocation pairs (defects of the plasma crystal). In the following part of the introduction, we will address various aspects of dislocations in colloidal and plasma crystals that are relevant to our investigation.

- In three dimensions, dislocations are high-energy defects, unlikely to be created by thermal fluctuations, but in two dimensions they are point defects, and pairs of dislocations such as dipoles with opposite Burgers vectors can be created easily [5]. (The Burgers vector characterizes the magnitude and direction of the crystalline lattice distortion by a dislocation.) In two dimensions, the dislocation can be constructed by inserting an extra half-line of atoms, i.e. a row of vacancies or interstitials [5, 7]. It is certainly a challenging issue to study the geometry of the coupled newly nucleated dislocations constituting a
cluster [8]. The nontrivial topology of the cluster is basically defined by the interaction between its components.

- The pair interaction between crystal dislocations was systematically explored recently by Eisenmann et al [9] for a crystal of magnetically interacting super-paramagnetic colloid particles on the surface of water. The results of this study on the whole confirmed that the standard Hamiltonian of the elastic dislocation theory allowed a quantitative understanding of the formation and interaction energies of dislocations in 2D crystals. The interactions of interstitials and vacancies in 2D colloidal crystals (with an $r^{-3}$ interparticle interaction potential) using Monte Carlo simulations have been studied in [10]. Modesto et al [11] have applied molecular dynamics simulation (with periodic boundary conditions) to study the energy of formation and interaction of vacancies in a 2D rare-gas crystal comprised of particles confined to two dimensions and interacting through a Lennard–Jones central pair-wise potential. DaSilva et al [12] have reported on the calculations of the formation energy of single-point defects and the interaction of pair-point defects in a 2D screened Coulomb interaction colloidal system. It has been pointed out that ‘...both the pairs of vacancy–vacancy and interstitial–interstitial are strongly attractive at short distances, with attraction going to zero for distances greater than three lattice spaces’. These distances are apparently much shorter than those computed for $r^{-3}$-interacting colloids; see [10]. The diffusive thermal motion of defects in a colloidal crystal has been considered by Libal et al [13].

- Using numerical and analytical calculations, the structure of vacancies and interstitials in 2D colloidal crystals for the special case of the Gaussian core model was studied by Lechner and Dellago [14]. The displacement fields predicted by elasticity theory were proven to be accurate at large distances, but large deviations occurred near the defect for distances of up to ten lattice spacings. The mobile defects can be treated as solitons; for example, Ablowitz et al [15] have found 2D solitons (Penrose solitons) in lattices possessing vacancy defects, edge dislocations and quasicrystal structures.

- The fact that the stable configurations of monovacancies, divacancies and interstitials have reduced symmetry compared to the hexagonal lattice has been verified in experiments with colloidal crystals by Pertsinidis and Ling [16]. (To suppress the out-of-plane motion, whence enabling a 2D structure, the aqueous suspension of 0.36 $\mu$m diameter polystyrene-sulfate microspheres has been confined between two silica substrates separated by $\approx 2 \mu$m.) The point defects, here monovacancies, divacancies and interstitials, were thermally excited forming separated dislocations, from which the authors extracted the dislocation pair potential.

- Not all questions have been resolved, however. Even to introduce the distance between two interacting dislocations in a pair is a challenging issue. In [9], for example, this distance is defined as the separation between the centers of every dislocation in the pair. (The center of the dislocation is introduced in [9] as the midpoint of the line joining fivefold and sevenfold coordinated particles.) For pure geometrical reasons this choice significantly narrows the angular distribution of dislocation positions in a pair, as has been observed [9]. In [17], on the other hand, the separation of two dislocations in a cluster is identified as the distance between two fivefold coordinated particles. The positions where the extra rows of particles terminate seem to be natural to use in measuring the inter-dislocation distances. In what follows, for identifying the dislocation positions, we adopt this convenient alternative.
• The geometrical properties of dislocations and dislocation clusters in colloids (in particular, the dislocation dipoles and dislocation pile-ups) were reviewed in [18]. A similar study has not been conducted for plasma crystals so far.

• Complex plasmas, i.e. low-temperature plasmas containing micron-sized particles [19, 20], allow investigations of many dynamical processes at the kinetic level, offering unique experimental perspectives. In complex plasmas where different kinds of phase transitions exist, e.g. in the electrorheological plasmas [21], one can find many examples of such studies. Nucleation of dislocations and symmetry alternation effects are naturally important in complex plasmas where the particle–plasma feedback mechanisms underlying many dynamical processes play an important role. Another option, interesting in many applications, is the clustering of a new phase which is asymmetric with regard to a background symmetry (for an example of a fluid phase separation in binary complex plasmas see [22]). A symmetry disordering escorting a crystalline–liquid phase transition in a complex plasma has been investigated experimentally in [23–26].

• Nucleation of clustered dislocations observed experimentally in a 2D complex plasma [23, 24, 27–29] is perhaps the simplest example of symmetry alternation effects. The dislocations are always nucleated in pairs inside the crystal (due to conservation of the Burgers vectors), and the tetragonal symmetry of the dislocation cluster cores is a striking counterpart of the otherwise hexagonal environment. In particular, it was observed [30, 31] that dislocations in plasma crystals appear to interact as dipoles, forming head-to-tail strings, or smaller structures where the dipoles are side by side with alternating orientations.

• Note that the vacancies in plasma crystals are also observed because of the ‘latent’ 3D structure of the complex plasma lattice layer. The vacancies are formed mostly by the ‘out-of-plane’ particles [23, 24], but might be manifested as ‘crushed’ (by nomenclature adopted from [16]) monovacancies as well, as is demonstrated in the given study.

• It is worth emphasizing that in the case of plasma crystals the interparticle interaction potential is of the screened Yukawa type, for which the typical interaction range (= the ratio of the lattice constant to the screening length) is known to be 0.5–2 [19, 20, 32]. Hence the particle interactions are much more compact in contrast to the \( r^{-3} \) interaction potential in the case of magnetically interacting colloid particles considered in [9]. Also the interactions are 3–10 times stronger than in the case of charged Yukawa-interacting colloid particles with an interaction range \( \approx 3 \) [16]. Thus there is a unique opportunity to verify whether the topology of the dislocation clusters is topologically universal.

The paper is organized as follows. Following this introduction (section 1), we formulate the main features of the simulation model applied (section 2), give an example of focusons, accompanying the twofold interstitial dynamics (section 3), discuss energetics and the displacement field of a single monovacancy (section 4), and then demonstrate deformation-induced nucleation in a hexagonal simulation cell specially constructed for this purpose (section 5). The topology of the thermally activated compact dislocation clusters and dumbbell interstitials is discussed in section 6. First a simple model of the point-like dislocations comprising a cluster core is formulated here. Then the statistical properties of the thermally activated dislocation clusters are studied. This gives us an opportunity to link the geometrical structure with the force field inside the cluster. In sections 4–6, the results of simulations are
also compared to the available experimental data. In section 7, the results obtained in the paper are summarized and the main conclusion is given.

2. Simulation features

2.1. A numerical model

To perform molecular dynamics simulations of a 2D complex plasma, we implement a ‘standard’ set of equations commonly used to describe the particle motion (see e.g. [31, 33–38]):

\[ m \ddot{r}_i = \mathbf{f}_{\text{ext}}^i + \sum_{j=1}^{N} \mathbf{f}_{\text{int}}^{i,j}, \quad i = 1, \ldots, N, \tag{1} \]

where \( m \) is the particle mass, \( \mathbf{r}_i \) the coordinate of the \( i \)-particle and \( N \) the number of particles. The first term to the right represents symbolically a sum of all possible external interactions, e.g. friction (external dissipation), \(-m \gamma \dot{r}_i\), due to collisions with neutrals (Epstein drag or neutral damping with a damping rate \( \gamma \)), excitation, ‘heating’ or confinement forces, whereas the second one describes mutual interparticle repulsive interactions via the Yukawa force,

\[ \mathbf{f}_{\text{int}}^{i,j} = \frac{q^2}{R^2} \frac{\mathbf{R}_{i,j}}{R} \left( 1 + \frac{R}{\lambda} \right) \exp \left( -\frac{R}{\lambda} \right). \tag{2} \]

where \( \mathbf{R}_{i,j} = \mathbf{r}_i - \mathbf{r}_j \) is the relative coordinate and \( R = |\mathbf{R}_{i,j}| \) is the distance between particles \( i, j \) with the coordinates \( \mathbf{r}_i, \mathbf{r}_j \); \( q \) is the particle charge and \( \lambda \) is the screening length. The latter two, \( q \) and \( \lambda \), following in our model from the simplest plasma/microparticles feedback mechanism, are assumed to be given constant parameters\(^2\).

Below we use \( \lambda \) as a space scale and

\[ \tau_Q = \sqrt{\frac{m \lambda^3}{q^2}} \tag{3} \]

as a time scale.

By applying a random force to each individual particle, a randomization (heating) is achieved. The requested kinetic temperature of the particle suspension is controlled by the amplitude \( A_{\text{heating}} \) of the employed random force and the counteracting frictional dissipation. The mean kinetic temperature can be estimated according to a very simple relationship (see e.g. [35, 38]):

\[ \langle K \rangle \propto \frac{A_{\text{heating}}^2}{\gamma}. \tag{4} \]

(The proportionality coefficient, not shown, depends on the parameters of the lattice layer.) This is actually a direct consequence of the fluctuation–dissipation theorem [39, 40]. Formally, there is no limitation on the dissipation rate in the model. Nonetheless, in what follows we assume that the frictional coupling is relatively weak, since it is important in our simulations to keep mutual particle interactions dominating. This situation can be realized in experiments too.

\(^2\) In numerous studies this simplified model has been proven to quite adequately describe the microparticle dynamics as detailed as necessary for the given study. Still it has to be noted that many important effects related to the microparticle charging, the non-Yukawa screening and the anisotropy and non-reciprocality of the particle–particle interactions determined by background plasma [20] are not included.
2.2. A hexagonal simulation cell

We observed that, to have a perfect structure, a given hexagonal cluster centered over one particle must contain exactly $N = 3S(S+1) + 1$ particles, where $S = 0, 1, \ldots$ is the number of fully packed hexagonal shells surrounding the center. For instance, an elementary hexagonal cell corresponds to $S = 1$; hence, $N = 3 \cdot 1 \cdot (1+1) + 1 = 7$ particles are involved in this elementary structure.

Following this simple rule we guessed that a defect-free hexagonal structure, having a size of $A = a(S+1)$, where $a$ is the interparticle distance, and containing exactly $N = 3S(S+1) + 1$ negatively charged particles arranged in $S$-shells, can be created when the particles are confined by a negatively uniformly charged ‘thin wire’ (of zero diameter) shaped as a hexagon and maintaining the confinement potential

$$
\varphi_{\text{ext}}(r) = \alpha \cdot \int_{\Gamma} \varphi_Y(R) \frac{d\Gamma}{\lambda}, \quad \varphi_Y(R) = \frac{q}{R} \exp \left( -\frac{R}{\lambda} \right), \quad R = |r - r'|.
$$

(5)

Here $\Gamma$ is a hexagon of size $A$, $\varphi_Y$ the Yukawa potential of a single point-like particle with charge $q$, and $\alpha$ the adjustable confinement parameter. This parameter controls evidently the charge density on the wire or, equivalently, the total charge on it. The confinement is effectively stronger at larger values of $\alpha$.

This assumption was confirmed in our simulations: running a series of simulations with repeating heating–recrystallization cycles, we assured ourselves that the particles are stably confined inside such a cell. It is worth noting that the use of confinement in a hexagonal well was investigated experimentally; see [41]. No rule exists enabling us to select the value of $\alpha$. All the simulations listed below have been performed choosing the value of $\alpha = 23$. Note that the cell design is similar to that implemented in [23] to simulate the melting and recrystallization process of the plasma crystal.

The simulation cell, as designed above, has the evident advantage of a flexible shape, compared to, e.g., a cell with parabolic confinement [38]. The cell geometry is easy to change by varying, e.g., the length of the sides or the position of the vertices (still keeping them connected), thereby obtaining a ‘deformed’ hexagonal shape. Deforming the boundary of the cell, it is easier to manipulate the particles in a tractable way. Below we have used this circumstance to demonstrate nucleation in simulations (see section 5.2).

An additional option of this flexible geometry is the opportunity to separate or consolidate pure shear and simple shear deformation [6] if desirable. The strain rate is controllable during the deformation as well. Examples of the parameter sets used in the simulations are collected in table 1.

2.3. Artificial introduction of defects

Another useful option, easily realizable within the hexagonal simulation cell, is the introduction of stable defects and defect clusters in a controllable way by manipulating the number of particles involved in the simulation. Following Kaski et al [7], it might be done by removing a part of a row of particles and allowing the rest to equilibrate, healing the crack created. As an illustration a few examples of the separated pairs and single perfect dislocations obtained are shown in figure 1.

The hexagonal cell designed as proposed is also very helpful in simulating dislocation clusters containing a vacancy or an interstitial. For instance, to create a vacancy it is enough to
Table 1. Plasma crystal parameters. The table accumulates the parameters of the experiments and numerical simulations cited in the figures. The simulations were performed making use of a hexagonal cell (section 2.2). $q$ is the particle charge, $m$ the particle mass, $\gamma$ the neutral gas damping rate, $\langle K \rangle$ the particle kinetic energy, $N$ the number of the particles, $\lambda$ the screening length, $a$ the interparticle separation and $\kappa = \frac{a}{\lambda}$ the interaction range.

| Experiment | Simulation | Figure | Reference |
|------------|------------|--------|-----------|
| 1 | | 11 | [51] |
| 2 | | | [23] |
| 3 | | 2, 9, 12 | |
| 4 | | | Given study |
| 5 | | | 23 |
| 6 | | | | Given study |

$a$ Averaged over the entire simulation run.

$b$ The initial value.

Figure 1. (Simulations) Artificial ‘nucleation’ initiated by cutting out a part of a row of particles (a, b) deep inside the cluster, or (c, d) with the cut extended to the crystal edge. The prepared configurations with the cuts were subjected to long-term equilibration. Note that the (a, b) configurations are dislocation dipoles with zero total Burgers vectors, whereas (c, d) are with non-zero Burgers vectors. The dislocations are immobile because there is not enough stress to overcome the Peierls barrier $\langle K \rangle \approx 0$. The black dots (connected with the tessellation lines) mark the particle positions inside the cluster. The defect cells are shown red (the sevenfold cells) and green (the fivefold cells).

remove a particle from its lattice site and wait until the lattice layer relaxes again. In experiments with colloids this has been done experimentally with the help of optical tweezers by Pertsinidis and Ling [16]. To create an interstitial, an extra particle has to be introduced at a desirable interstitial position. In simulations the vacancies and the interstitials in colloids were studied recently by Lechner and Dellago [14].
Figure 2. Configurations of monovacancies in the 2D plasma crystals (a–c) extracted from data obtained in the experiments by Knapek et al [23] and (d–f) ‘synthesized’ in simulations of the given study. By nomenclature from [14, 16, 17]: (a, d) split (SV); (b, e) twofold crushed monovacancy ($V_a$); (c, f) threefold symmetric monovacancy ($V_3$). The black dots label the particle positions inside the cluster. The black lines indicate the particle connections obtained with the standard Delaunay triangulation routine\textsuperscript{3}. The defect cells are colored as follows: eightfold, blue; sevenfold, red; fivefold, green. These configurations, except for evidently different topological arrangements, can be distinguished, e.g., by binding energies.

A few examples of the vacancies and interstitials simulated in the given study and/or experimentally observed in complex plasmas are shown in figures 2–4 and 9. These defects in 2D plasma crystals are shaped similarly to those in 2D colloids. Topologically this universality is actually not surprising. Nonetheless, there is an important symmetry feature allowing us to distinguish point defects ‘made’ in colloids or synthesized in complex plasmas: the dislocation clusters in the plasma crystals appear to be more compact (being scaled with the lattice distance, of course; the physical size of defects and defect clusters in colloids is normally smaller).

The defect clusters formed in the vicinity of a vacancy or interstitial might be quite developed before they reveal the internal symmetries of the defect clusters. For example, chirality effects and the mirror-symmetric structures can be observed. In that sense there is a certain resemblance between the defect cluster symmetries and the chirality of some organic molecules [1]. A couple of the examples obtained are shown in figure 3. We will save this very interesting development for forthcoming detailed research.

\textsuperscript{3} The Delaunay triangulation routine, the standard application, e.g. in Mathematica version 5.1.1, is convenient to use; as an example of the triangulated particle positions obtained, see e.g. figure 1.
3. Mobile interstitials as ‘focusons’

An interesting opportunity appears if one introduces two new closely positioned particles to interstitial places in the lattice layer. At a general position this initiates a localized distortion, quite rapidly relaxing and forming a twofold interstitial, e.g. like those shown in figures 3(a) and (b).

The relaxation process was eventually different when the positions of ‘intruders’ were chosen exactly in-row along one of the main crystal axes. The anisotropy in particle displacements (dominantly in one of the three high-symmetry axes of the crystal) for the $I_2$ interstitials has been noted for the first time by Lechner et al [42]. The interstitials created were unusual in form (two sevenfold particles clustering with a fourfold one) and behaved strangely: they moved unbroken quite a long distance in opposite directions as if they repelled each other; see figure 4. (The Burgers vector of every defect group in figure 4 is evidently zero.) This unusual behavior is easy to explain by the mutual repulsion of the core particles, enabling a cascade of focused collisions—‘focusons’ [45]—propagating along the rows of the closed packing. (Newton’s cradle might serve as a good analogue of the momentum transport in focusons.) Focusons have also been observed in experiments [46].

It is evident from figure 4(a) that the interstitial mobility has a peculiar stick-and-slip character: quite smooth periods of motion of the cluster as a whole, accompanied by the rearrangement of its components, are suddenly replaced by the ‘quantized’ jumps of the cluster center of mass to the new position. The latter, the equidistant jumps, is a direct consequence of the discreteness of the particle positions in the crystal.

4. Simulated threefold symmetric monovacancy

Next, as a more detailed example, let us consider the special case of the threefold monovacancy. To create this vacancy formation, a central ‘atom’ was eliminated from a pre-prepared well-equilibrated crystal cluster (for the simulation parameters, see case 4, table 1). The defect cluster, appearing around this vacancy (like that shown in figure 2(f)), is marvelously symmetric, and hence simple. It readily helps to avoid unnecessary complications arising from the initial asymmetry.
Figure 4. (Simulations) The introduction of two particles symmetrically along a row of dense packing leads to the formation of mobile defect groups formed by focusons (focused collisions, see e.g. [45]). (a) The lines are the trajectories (cyan) of the fourfold cells (centers of the dislocation clusters) and (red) of the ‘accompanying’ sevenfold cells. The cluster cores are stable; their size slightly increases (up to a maximum of \( \sim 15\% \)) with a weak oscillation (\( \sim 2–5\% \)) during propagation. The inset shows the clusters’ position at \( t/\tau_Q = 1 \) (as indicated by the vertical dashed line). (b) The kinetic energy distribution at \( t/\tau_Q = 3 \). The focusons are seen as two sharp peaks in the kinetic energy distribution. They are followed by the defect groups constituted from (stars) the fourfold cells and (red triangles) the sevenfold cells.

4.1. Dynamics of the displacements’ field

A cascade of the dynamic nucleation process is demonstrated in figure 5. Nucleation of the vacancy happens to be a multi-scale dynamical process, as can be seen from the mean kinetic and potential energy variations (figures 5(a) and (b)). A rough sequence of the events is as follows: after a relatively short initiation stage, comprising relatively strong accompanying oscillations, the entire cluster relaxes first into a perfectly symmetric intermediate phase A (figure 5(c)). This phase appears to be metastable and, being sufficiently disturbed (by a computation imperfection), passes to a more stable state of equilibrium, phase B (figure 5(e)). The temporal growth in the kinetic energy in the end of phase A, see figure 5(a) (and a consequent drop in the potential energy, figure 5(b)), is a key signature of the transformation. The involved short-time oscillations, stemming from the caged character of the particle motion, are easy to identify as well.

The initial and resultant configurations of the ‘atoms’ shown in figures 5(c)–(e) are depicted by using two different colors to distinguish them. The displacement field for the phase A vacancy is azimuthally symmetric (see figure 5(c)), whereas the displacements vary azimuthally in the phase B vacancy (with respect to the cluster geometric center, figure 5(e)). We introduce the displacements as the difference between the current \( \{ \mathbf{r}_i(t) \} \) and the initial \( \{ \mathbf{r}_i(0) \} \) particle...
Figure 5. (Simulations) Nucleation dynamics of a single vacancy triggered by removing a central particle from the cluster of 631 particles, showing the variation of the kinetic energy (a) and the potential one (b) of the entire cluster during the equilibration process. The dashed lines in (a) and (b) indicate an exponential decay (the same in both cases): $500 \exp(-\gamma t)$ [eV]. The phase A metastable vacancy (c) and the phase B stable vacancy (e) are as revealed by the particle displacements: from the initial positions (black dots) to the subsequent ones (red dots); (d, f) show the particle displacements versus normalized radius $R/\lambda$. The dashed lines in (d) and (f) are the exponents $D = 0.15\lambda \exp(-\frac{R}{\lambda})$, where $L = 2\lambda$ is the spatial decrement. The insets (enlarged) show the actual structure of the defects, colored for better visibility. The time moments (nucleation starts at $t = 0$) are: (c, d) $\frac{t}{\tau_0} = 8$; (e, f) $\frac{t}{\tau_0} = 24$. The breathing-type oscillations of the entire cluster at a frequency of $\simeq 4$ Hz are also noticeable ((a), (b); $\frac{t}{\tau_0} > 10$).
configurations by
\[ D_i(t) = |\Delta r_i|, \quad \Delta r_i = r_i(t) - r_i(0). \] (6)

Although the asymmetry is immediately evident from the particle positions, it does not cost too much energetically: the energy gap between the phase A and the phase B configurations is only \( \Delta U_{A\to B} \approx 11.2 \text{ eV}. \) Another prominent feature is that the proximity of the phase A vacancy is a nearly perfect hexagon with all interior angles \( \simeq 120^\circ \). By general definitions it is a regular polygon which can be either circumscribed or inscribed. The proximity of the phase B vacancy is more peculiar, and not all the interior angles are the same: three of them, related to the fivefold cells, are smaller, \( \simeq 113^\circ \) each, and the rest, connected to the sevenfold cells, are of \( \simeq 127^\circ \). This polygon cannot be circumscribed but can be inscribed by a circle, which helps to imagine the deformation involved.

Both configurations are surprisingly compact; the displacements decay exponentially away from the origin, \( \frac{D}{\lambda} \propto \exp(-R/L) \), where \( R \) is the radius and \( L \simeq 1.8 \text{ mm} \) is the spatial decrement. This can be clearly seen in figures 5(d)–(f), where the displacements of all cluster particles are plotted versus their radial positions (shown are states at two fixed time moments). This is a distinguishable feature, for colloids, e.g. the displacements decay over a distance \( r \) slower, i.e. as \( r^{-1} \) [14].

The spatial decrement of the symmetry alternation is quite short \( L \simeq 2\lambda \), that is, over three lattice constants only. The spatial decrement was estimated from the slope of the displacements’ radial dependence (see figures 5(d)–(f)). It is important to also mention that the distortion region is only a small part of the entire cluster. (The size of the latter is approximately ten lattice constants in the given simulation run.) Therefore, the boundary effects are not a trouble at all, at least at distances of three lattice sites away from the boundary.

4.2. The compactness of a monovacancy

Figure 5 shows that the compact clusters do form preferentially. This important message is especially worth addressing: the compactness of the vacancy cluster violates the ‘standard’ elasticity theory expectations, predicting a long-range displacement field.

Note that the long-range character of the point defect field stems directly from the basics of the ‘standard’ plasticity theory based on the Green’s function machinery; see Pellegrini [47] for one of the most recent reviews. (The true advantage of this approach is the ability to restore, let it be just in principle, the induced distortions produced by inclusions or defects in their surrounding medium [47].) In the simplest isotropic static limit, for instance, the Green’s function of the elastic displacements is [47]

\[ G_{ij}(k) = \frac{1}{\mu k^2} \left[ \delta_{ij} - \frac{1}{2(1-v)} \frac{k_i k_j}{k^2} \right], \] (7)

where \( k \) is the wave number, \( \delta_{i,j} \) the Kronecker symbol and \( \mu \) and \( v \) the shear modulus and Poisson’s ratio. The latter are convenient to introduce through the shear \( (c_S) \) and longitudinal \( (c_L) \) sound velocities, measured directly in plasma crystal experiments (see e.g. [48]),

\[ \mu = \rho c_S^2, \quad v = \frac{1}{2} \frac{1-2p}{1-p}, \quad p = \frac{c_L^2}{c_S^2}, \quad \rho = \frac{2m}{\sqrt{3}a^2}, \] (8)

where \( \rho \) is the area density of the lattice layer.
The fact that the point defect has to form a long-range tail of displacements follows readily from the relationship (7): \( G \propto k^{-2} \rightarrow \infty \) at \( k \rightarrow 0 \). Such a kind of a long-wavelength ‘catastrophe’ leads to a logarithmic singularity of the Green’s function in real space and, in turn, to \( D \propto r^{-1} \) asymptotics in the displacements [14].

The situation in the case of the plasma crystals is not usual. First, it is worth noting that in experimental plasma crystals \( p \approx \frac{1}{2} \), \( c_l^2 \ll 1 \). This implies that \( v \approx \frac{1}{2} (1 - p) \approx \frac{1}{2} \). Therefore the plasma crystals, being a soft material in view of the extremely low elastic moduli, are nearly incompressible in the elasticity sense. (Note that the sound velocities estimated with the help of [50] are \( c_L = 27.0 \text{ mm s}^{-1}, c_S = 3.8 \text{ mm s}^{-1} \) for given simulation conditions.) Next, it is reasonable to guess that the confinement (or an effective ‘quasi’-confinement) effect could be important in explaining the compactness of the vacancy in the plasma crystal. A finite confinement is expected to change the Green’s function’s divergency character and, as a consequence, to change the power-law asymptotics in displacements to the exponential one, in analogy with [38] where the influence of the weak global confinement on the crystal structure was studied.

In the case of a vacancy, an additional stronger confinement might appear self-consistently provided by a compression of the vacancy core by the surrounding particles. The confining field distribution can be computed directly by summing up the contributions of the particles surrounding the core. For the ‘newly born’ vacancy, e.g. the obtained confinement well profile in the vicinity of the vacancy center turned out to be practically isotropic (within an anisotropy \(< 3\% \)) and approximately parabolic (within an inaccuracy \(< 10\% \)):

\[
\delta U^{sc}(r) = \frac{1}{2} k^{sc} r^2, \quad \frac{r}{\xi} < 0.6, \quad (9)
\]

where \( r \) is the distance to the center and \( k^{sc} \approx 1.85 \text{ KeV mm}^{-2} \) is the string constant.

This observation is easy to address, e.g. in the mean-field approximation, by replacing the real crystal layer containing a vacancy with a charged disc with a hole in the center. Let us denote by \( r_h \) the hole radius and by \( \sigma^{mf} = q n_{hex} \) the disc charge density. (Here \( n_{hex} = \frac{2}{\sqrt{3} a^2} \) is the density of the hexagonal lattice layer and \( a \) is the lattice constant.) It is elementary to calculate the disc field and compute the potential energy of a charge \( q \) placed in the hole close to the disc center,

\[
\delta U^{mf}(r) = \frac{1}{2} k^{mf} r^2, \quad k^{mf} = \frac{2 \pi q^2}{\sqrt{3} \lambda a^2} \left( \frac{1 + \xi}{\xi} \right) e^{-\xi}, \quad \xi = \frac{r_h}{\lambda}. \quad (10)
\]

From the balance \( k^{mf} = k^{sc} \), it follows that the hole radius has to be \( \frac{r_h}{\lambda} \approx 1 \). The hole radius is greater than the lattice constant \( \frac{a}{\lambda} = 0.65 \) and still less than the vacancy size \( \frac{L}{\lambda} \approx 2 \) (see figures 5 and 6).

More evidence that the confining well can be treated as parabolic originates from the counterbalance of the local confinement force \( F_r^{sc}(r) = -\partial_r \delta U^{sc}(r) = -k^{sc} r \) and the mutual repulsion forces acting on a particle in the vacancy core:

\[
F_r^{core}(r) = \frac{q^2}{r^2} \left[ (\varrho + 1) e^{-\varrho} + \frac{1}{4} (2 \varrho + 1) e^{-2\varrho} + \left( \varrho + \frac{1}{\sqrt{3}} \right) e^{-\sqrt{3} \varrho} \right], \quad \varrho = \frac{r}{\lambda}. \quad (11)
\]

(It is assumed that the six core particles are roughly evenly distributed at the core radius.) From the balance \( F_r^{sc}(r) + F_r^{core}(r) = 0 \), it is straightforward to estimate the core radius \( \frac{r}{\lambda} \approx 0.6 \), in good agreement with simulations, giving approximately the same mean radius of the vacancy core \( \langle \frac{r}{\lambda} \rangle \approx 0.56 \) for both phase A and B configurations (see figure 5).
Figure 6. (Simulation) The particle displacements inside the vacancy core obtained with a cluster containing initially (black dots) \( N = 631 \) and (red dots) \( N = 1519 \) particles (table 1, cases 4 and 6; \( \frac{L}{\tau_0} = 20 \)). The spatial decrement is the same as in figure 5. The \( R^{-1} \) profile is shown for comparison.

Finally, it is especially worth noting that there is no contradiction to have an equidistant lattice constant—this is merely an advantage of our simulation technique (see section 2), having a pretty flat external confinement in the cluster center—and the strong local ‘self-confinement’ well due to the vacancy.

4.3. The energy costs

In our case the dust-background gas collisions are responsible for the friction losses. Taking it into account, the potential energy change \( \Delta U \) of the lattice layer due to the vacancy can be estimated from the energy balance

\[
\Delta U = A_{fr}, \quad U = U_{int} + U_{ext}, \quad A_{fr} = -2\gamma \tau_{eq} \langle K \rangle, \tag{12}
\]

where \( U_{int} \) is the potential energy of the particles’ mutual interactions, \( U_{ext} \) the potential energy of the external confinement, \( K \) the kinetic energy, \( A_{fr} \) the negative work of the friction forces and \( \tau_{eq} \) the equilibration time. The potential energies and the kinetic energy are introduced as

\[
U_{int} = \frac{1}{2} \sum_{i \neq j} q \varphi_{ij}(R_{i,j}), \quad U_{ext} = \sum_i q \varphi_{ext}(r_i), \quad K = \frac{1}{2} \sum_i m r_i^2, \tag{13}
\]

with the sums running over all particles.

For the vacancy nucleated in the cluster center, the simulations (for the simulation parameters, see case 4, table 1) show that \( U_{ext} \) does not exceed approximately 17% of the total potential energy. Nonetheless, the external confinement forces play an important role in the process of nucleation. For example, the energy variations taken over the whole equilibration period are

\[
\Delta U = A_{fr} = -191.5 \text{ eV}, \quad \Delta U_{int} = 192.8 \text{ eV}, \quad \Delta U_{ext} = -384.3 \text{ eV}.
\]
One can see that the work of the external forces is divided approximately equally among friction energy, loss and configuration energy. In the absolute value, compared to the configuration energy, it is twice as large.

Another interesting observation is the fact (see figure 5) that at a sufficiently large scale the potential and the kinetic energy variation decay exponentially during nucleation:

$$\delta U \simeq \delta K \sim K_0 e^{-\gamma t}, \quad K_0 = 500 \text{ eV}. $$

The equipartition of the energy variations, the kinetic and the potential, is usually treated as a consequence of the virial theorem. It is worth noting that the virial itself

$$V = V_{\text{int}} + V_{\text{ext}}, \quad V_{\text{int}} = \frac{1}{2} \sum_{i \neq j} R_{i,j} f_{i,j}^{\text{int}}, \quad V_{\text{ext}} = \sum_i r_i f_i^{\text{ext}},$$

(14)
decreases, as it is easy to show, at twice the lower rate, $|V| \sim e^{-1/2 \gamma t}$. It follows readily from the exact relationship valid for our dynamical system:

$$\ddot{J} + \gamma \dot{J} = 2V + 4K, \quad J = \sum_{i=1}^{N} m r_i^2.$$  

(15)

Here, $J$ is the momentum of inertia of the entire particle cluster with respect to its geometrical center at $x = y = 0$.

5. The complexity of dislocation clusters’ nucleation kinetics

5.1. Nucleation of dislocation clusters in plasma crystals

Irrespective of any detailed melting scenario, the question of what mechanism explains nucleation of the primary dislocations remains. Recently, this issue was studied experimentally: spontaneous nucleation of the edge-dislocation pairs (followed by their dissociation) has been successfully observed at the kinetic level in experiments with plasma crystals [28]. The dislocation pairs were created in the lattice locations where the internal shear stress exceeded a threshold. It has also been shown that even an elementary act of nucleation is in fact a multi-scale process consisting of the latent ‘pre-phase’, the prompt nucleation of a defect cluster and the dissociation of the cluster followed by the escape of free dislocations [51]. To survey such detailed dynamics in real time is a true advantage of experiments with plasma crystals.

Since the Burgers vector of the entire lattice is kept constant (e.g. zero), spontaneously created dislocations must appear in clusters with a zero Burgers vector. In the simplest case they are defect quadruplets of the type $(\delta z, \delta z)$. Such cramped topological configurations we denote as compact dislocation clusters. Note that most of the dislocation clusters observed in complex plasma crystals appeared to be compact. They have to be distinguished from the crushed monovacancies (using the nomenclature adopted in [16, 17]), the dislocation pairs surveyed in colloidal crystals with a Yukawa-type interaction, and from the dumbbell interstitials, studied numerically in [14] for the colloids with a Gaussian interaction. All those defects are exhibited by a pair of coupled dislocations but inherently different configurations; see, e.g., figures 2, 3 and 9.

As is well known, a single straight dislocation cannot be formed within a crystal by localized glide motions. The formation of a pair of edge dislocations of opposite signs on the same glide plane was considered by Nabarro [44]. This system cannot be in stable equilibrium,
but if a shear stress is applied to the crystal it is possible to find a position of unstable equilibrium in which the attraction between the dislocations balances the force with which the applied stress tends to separate them [44]. Therefore, compact clusters are necessarily meta-stable objects; their lifetime depends on the temperature or the stress applied.

5.2. Simulation of deformation-induced nucleation

In the experiments [28, 51], it was suggested that the stress that finally caused nucleation was affected by the differential crystal rotation. The exact reason for nucleation, however, was difficult to determine consistently. In simulations the nucleation conditions are certainly easier to identify. For instance, figure 7 shows a simple-sheared particle lattice layer. At a properly chosen loading rate the deformation causes a shear instability that ends up with nucleation of defect clusters in the bulk of the lattice layer. After a while, when the deformation becomes stronger, the components of the clusters decouple and the newly born free dislocations glide away in a similar manner to the dislocations observed in experiments.

The hexagonal simulation cell (see section 2.2) contains 631 equally charged particles interacting pair-wise via the Yukawa (the screened Coulomb) force. The forces, deforming the cluster, are applied from left to right on top of the cell, and from right to left on the bottom. The central horizontal line of the cell is kept non-deformed. The deformation rate is \( \tau Q \ddot{\epsilon} = 0.05 \), \( \tau Q \simeq 0.12 \, s \), where \( \tau Q \) is the Coulomb time scale introduced by relationship (3) and \( \epsilon \) is the shear strain [6]. The simulation parameters are listed in table 1 (case 4).

Symmetry breaking, the mechanism accompanying the shear instability, is of primary importance for understanding the nucleation of dislocation clusters. The stable configurations of defects, likewise observed in colloids [16], have reduced symmetry compared to the otherwise hexagonal environment and a peculiarly structured topology. We discuss this important issue below in section 6. Note also that plastic deformations of complex plasma crystals under
slow uniaxial compression, accompanied by nucleation of dislocation pairs, were studied experimentally and numerically recently by Durnak and Samsonov [29].

5.3. Dislocation and dislocation clusters in a recrystallizing complex plasma

One of the possible scenarios for melting (recrystallization) in a 2D complex plasma is a steep increase (decrease) in the density of the dislocations and the dislocation aggregates (such as defect clusters, grain boundaries, etc) [52, 53]. To study this scenario in simulations, it is desirable to avoid any complications associated with the lattice layer sectioning ‘from the very beginning’ [38]. A promising tool in that sense, allowing a defect-free initial lattice layer, is the hexagonal confinement cell proposed in section 2.2.

Simulations showed that not only isolated pairs, dislocations \((s^7)\), but also compact triplets such as \((s^7s)\), quadruplets \((s^7s^5)\), etc, or even elongated defect chains were quite frequent. Actually they dominantly defined the symmetry of the entire particle suspension at higher temperatures (see also [31]). It would certainly be interesting to connect the cluster formation in ordered complex plasmas [20] with the general percolation process known in many similar applications (see e.g. [54, 55]).

In such melted clusters, in agreement with recent experimental observations [23, 24, 53], the defect density permanently decreased upon cooling. At higher temperatures at the beginning of the recrystallization process, while the mutual interparticle collisions were still frequent, the defect density dropped exponentially, suggesting an Arrhenius-type, quasi-equilibrium disorder (see figure 8).

Then, at lower temperatures, stable defect clusters appeared, the decay rate significantly slowed down, and the quasi-equilibrium Arrhenius-type decay is replaced by a power-law decay. The appearance of clusters (collective order) resulting from the spontaneous breaking of discrete symmetry produced by short-range dislocation interaction is analogous to that discovered within the Ising model [56–59].

A sharp drop in the defect numbers followed by a quasi-saturation resembles the well-known situation [60] in which both thermal activation and tunneling events occur. Hence, by analogy, the fact that in our case the system of defects behaves in a similar way could be naturally explained by an annihilation scenario which is presumably of the dissipative tunneling type [60, 61] at lower mean kinetic energies.

6. Compact dislocation clusters

6.1. A remark on the processing procedure of dislocation clusters

First a few words on how dislocation clusters were analyzed. The dislocation tracking procedure is well developed (see e.g. [9, 23, 24, 28] and references therein). Either in experiments or in simulations this procedure starts from tracking—identifying particle positions [49]. The set of particle coordinates elucidated is then subjected to the standard tessellation procedure, which is carried out by joining all points, i.e. particles [62]. The tessellation routine provides the convex hull and the list of nearest neighbors (see footnote 3).

In the original hexagonal structures, most particles have six neighbors, form sixfold cells, and hence their coordination numbers \(n = 6\). All cells having \(n \neq 6\) are treated as defects. Simple sorting by coordination numbers gives a list of defect cells. Some of the defect cells...
Figure 8. (Simulations) Dislocation density versus inverse mean particle kinetic energy. The dashed line is the least-squares fit to the Arrhenius-type dependence $N_{\text{disl}}/N = A \exp(-Q/\langle K \rangle) + B$ plotted with $A = 0.12$, $B = 0.037$, $Q = 3.3$ eV. (For comparison: the activation energy $Q = 2.4$–$2.6$ eV has been measured in [53].) The initial exponential drop in the number of dislocations is clearly seen at $\langle K \rangle^{-1} < 2$ eV$^{-1}$. Next, at higher $\langle K \rangle^{-1}$, the exponential decay is replaced by a power-law decay [23, 24, 53]: in the figure $N_{\text{disl}}/N \approx \text{const}$ due to the narrow range of the inverse mean kinetic energies involved. The cluster was heated until a mean particle kinetic energy of 10 eV was reached and then the heating source was switched off. The simulation parameters were chosen to match the recrystallization experiment [23, 24].

are joined. Among them the doublets ($\xi^7$) or ($\gamma^5$) are identified as dislocations. Checking for the joined cells in question is the next evident step, enabling the primary list of dislocations.

Searching for compact dislocation clusters means seeking joined dislocations. To give an idea of what this implies, we recall that any compact dislocation cluster is a quadruplet of the type ($\xi^7 \gamma^5$) where the sevenfold cells are closer to each other than the fivefold ones. It has a quadrilateral in the core formed by the centers of the fivefold and the sevenfold cells, constituting the cluster. Hence, the searching procedure is equivalent to examining whether the pairs of dislocations have a common core, which is again an elementary sorting operation.

Compact clusters are easy to distinguish from other species. For instance, a dumbbell interstitial is also constituted by two dislocations, but they are arranged differently as ($\gamma^5 \xi^7$) with the fivefold cells closer to each other, which allows us to trace these defects separately. Some of the parameters obtained are collected in table 2. The searching procedure is equally applicable to data collected in either simulations or experiments. A few examples of the tracked dislocation clusters are reproduced in figure 9.

6.2. Geometry of the cluster core

The compact cluster—the dislocation dipole [18] (or short-vacancy dipole [5]) design is mixed in the sense that the hexagonal symmetry of the particle system (figure 9) neatly turns into
Table 2. Dislocation dipole cluster parameters from experiments and simulations. $K$ is the particle kinetic energy, $U_Q = \frac{q^2}{\lambda}$, $\tau_Q$ the Coulomb time scale, $\tau_{cc(di)}$ the compact cluster (dumbbell interstitial) lifetime, $\langle \Delta U_{cc(di)} \rangle$ the mean core configuration energies and $\delta d_{cc(di)}$ the shape factors, 20. (cc $\equiv$ compact clusters; di $\equiv$ dumbbell interstitials.)

| $q$ (10$^3$e) | $\lambda$ (mm) | $\langle K \rangle$ (eV) | $U_Q$ (keV) | $\tau_Q$ (ms) | $\langle \Delta U_{cc(di)} \rangle$ | $\langle \Delta U_{cc(di)} \rangle$ (max) | $\delta d_{cc(di)}$ | $\delta d_{cc(di)}$ (%) |
|---------------|----------------|-----------------|-----------|---------------|-------------------------------|---------------------------------|----------------|----------------|----------------|
| 1             | 15.0           | 0.44            | –         | –             | 26                           | –                               | –               | 10             | –               | –               |
| 2             | 13.0           | 0.75            | 0.4–1.6   | 0.32          | 82                           | 3.16                            | 2.94             | 5.6$^b$        | 4$^b$          | 8               | 69              |
| 3             | 13.0           | 0.75            | 1.5–8     | 0.32          | 82                           | 3.27                            | 3.14             | 2.2$^c$        | 4.5$^c$        | 13              | 71              |

Experiment

| 4             | 14.4           | 0.66            | 7.3       | 0.45          | 61                           | 2.03                            | 1.98             | 3.1$^d$        | 2.6$^d$        | 12              | 70              |

Simulation

- $\langle \tau_{cc} \rangle \approx 1.2$, $\langle \tau_{cc} \rangle \approx 1.3$, $\langle \tau_{di} \rangle \approx 0$.
- $\langle \tau_{cc} \rangle \approx 0.5$, $\langle \tau_{cc} \rangle \approx 0.4$, $\langle \tau_{di} \rangle \approx 0$.
- $\langle \tau_{cc} \rangle \approx 0.7$.

$^a$For the clusters shown in figure 11.

$^b$For the clusters shown in figure 11.

$^c$For the clusters shown in figure 11.

$^d$For the clusters shown in figure 11.

Figure 9. The compact clusters and the dumbbell interstitials (a, b) recovered from the experimental data [23] and (c, d) simulated (the given study) in a 2D complex plasma for the configurations (a, c) of the compact clusters and (b, d) the ‘dumbbell’ interstitials.

a nearly tetragonal symmetry of the cluster core. The stress fields of the components almost cancel far from the dipole [18]. Despite the apparent simplicity of the cluster interior—only four nearest neighbor particles, the centers of the five- and sevenfold cells, are in the core—to discover the cluster topology and binding energy is certainly a challenge, and the results are not as predicted by elastic theory [5].

In ideal 2D monolayers, dislocation dipoles are greatly favored and are tightly bound, behaving as single, immobile defects [5]. A favored generation of dipoles was also the case in our simulations and experiments. The high generation rate of the dipoles allowed us to closely explore the topology of these agglomerated defects in simulations. In the course of the simulations the particles are kept at a fixed mean kinetic energy high enough to provide...
nucleation of dislocations, \( \langle K \rangle = 7.3 \pm 0.2 \text{ eV} \). (The simulation parameters are listed in table 1, case 3.) The simulation time is \( \Delta t / \tau_Q = 120 \), \( \tau_Q = 0.061 \text{ s} \). The integration time step was chosen to be small enough, \( \delta t / \tau_Q = 0.04 \), to ensure a stable simulation.

Using simulation data, we traced the dislocation clusters as was explained above (see section 6.1). The main results of this study are as follows. The centers of the fivefold cells compose a nearly regular compact tetragonal structure, which is a bit squeezed by the environment. The mean size of the cell edges is \( \langle s \rangle \equiv 1/4 \langle p \rangle = (0.96 \pm 0.04) a \), where \( \langle p \rangle \) is the mean cell perimeter and \( a = 0.66 \text{ mm} \) is the lattice constant.

To explore more closely the topology of the core of a dislocation cluster, it is convenient to reorient all traced clusters. This can be done, e.g., by performing a rotation operation:

\[
z' = R \cdot (z - z_{cm}),
\]

where

\[
R = \frac{z_{1}^{(5)} - z_{2}^{(5)}}{|z_{1}^{(5)} - z_{2}^{(5)}|}
\]

is the rotation operator, and

\[
z_{cm} = \frac{1}{4} \sum_{k=1,2} [z_{k}^{(5)} + z_{k}^{(7)}]
\]

the center of mass of the cluster. Here \( z_{k}^{(5),(7)} = (x + iy)^{(5),(7)} \) are the complex coordinates of the five- and sevenfold cells, respectively, and \( i \) is the imaginary unit. This procedure revealed whether the simulated dislocation clusters have an orientational trend inside the otherwise hexagonal environment. Actually they do not, as the results of our simulations showed. Likewise in the case of colloidal crystals [9], there is no remarkable preferential orientation (figure 10).

To obtain an idea of the core topology, let us start with a simple model treating the cluster as constituted by two point-like dislocations, which are set apart at a distance \( r \) and allowed to glide only along two fixed crystallographic planes separated by one lattice period \( a \), so that

\[
r \equiv a / \sin \varphi,
\]

where \( \varphi \) is the angle of mutual orientation of the cluster components with respect to the gliding plane. The interaction energy of the point dislocations having the counter-directed Burgers vectors is [9, 63–65]

\[
u_{dd}(r) = \frac{2}{\pi \sqrt{3}} M c^2 r \left[ \frac{\ln \left( \frac{r}{a} \right)}{r^2} + a^2 r^2 \right] + \text{const.}
\]

It has a minimum, a stable ground state, at \( r / a = \sqrt{2} = 1 / \sin \varphi \). This corresponds to \( \varphi = 45^\circ \); hence the tetragonal symmetry of the cluster core might be considered as preferred. Actually, this is a well-known classical result in the continuum theory of dislocations [18]. It is only questionable whether it is applicable so straightforwardly to the study of compact clusters. Nonetheless, this prediction agrees surprisingly well with the results of simulations of finite clusters: on average the edge-to-diagonal angle in the compact cluster core appears to be \( \langle \varphi \rangle = 42^\circ \pm 2^\circ \).

It is also worth noting that the lengths of the diagonals of the core quadrilateral are different \( \langle d_{5-5} \rangle \simeq 1.43 \), \( \langle d_{7-7} \rangle \simeq 1.27 \) (see figure 11). As the shape factor, it is convenient to introduce the ratio of the diagonal lengths difference to the mean diagonal length

\[
\frac{\delta d}{\langle d \rangle} = 2 \frac{\langle d_{5-5} - d_{7-7} \rangle}{\langle d_{7-7} + d_{5-5} \rangle},
\]

(20)
Figure 10. Patterns of orientational preference of the dislocation clusters obtained in simulations. (Black dots) The cell positions revealed a visible ‘quasi-hexagonal’ trend in orientations for (a) the sevenfold and (b) the fivefold components of the clusters. The mean positions are indicated by blue and red dashed lines. The mean radii are $R_7 = 0.636a < R_5 = 0.714a$.

Despite the fact that the distances $\langle d_{7-7} \rangle$, $\langle d_{5-5} \rangle$ are quite distinguishable, the relative variation of the shape factor, e.g. for the compact clusters, is rather small $\delta d_{cc} \langle d \rangle \approx 0.12$. This means that the compact cluster core is nearly cyclic. A measure follows from the famous Ptolemy’s inequality valid for any quadrilateral:

$$Pt \equiv \frac{s_1s_3 + s_2s_4}{d_1d_2} \geq 1,$$

where $s_1, s_2, s_3, s_4$ denote the (ordered) sides, and $d_1, d_2$ are the diagonals of the quadrilateral. Over 80% of the recognized compact clusters have $1 \leq Pt \leq 1.03$ for the simulation results. For comparison, a hexagonal four-side cell (rhombus) corresponds to $Pt^{\text{hex}} = 2/\sqrt{3} = 1.1547$. The cores of the dumbbell interstitials are evidently not cyclic. The dislocation clusters taken from the experiment (see table 1) were processed in the same manner as the simulated ones. The results obtained are reproduced fairly well in simulations; see table 2.

6.3. Configuration energy and the cluster lifetime

Note also that a stable defect cluster could not be obtained by only shifting the positions of four central particles from the hexagonal configuration to the tetragonal one. Such a deformation would be reversible and hence unstable. A weakly deformed environment, the impeding relaxation of the core particles back to the stable hexagonal configuration, is indeed a necessary ‘lock’ making the deformation plastic, i.e. irreversible [44].

The topological arrangements of the core particles shown in figures 10 and 11 can be interpreted slightly differently. From the statistics of the core elements, in principle one can
Figure 11. The topology of a compact cluster core. (a) Normalized and reoriented centers of the fivefold (A, C, red dots) and the sevenfold (B, D, blue dots) cells compose a nearly regular compact tetragonal structure. The black quadrilaterals represent a few superimposed experimental clusters taken from [28, 51] and shown for comparison. (The experimental data points were normalized by $a_{\text{exp}} = 0.69 \text{mm}$ to adjust a scaling factor.) (b) The occurrence histogram shows that in the cores, $d_{55}$-diagonals are systematically larger (over 8% on average) than $d_{77}$-diagonals, $AC > BD$. Nonetheless, the distributions remarkably show the same variances, $\text{Var}(d_{77}) \simeq \text{Var}(d_{55}) \simeq 0.086a^2$.

eucidate the force field maintained inside the cluster interior. To get an idea of the scale of the energies involved, we computed the distribution of the dipole cluster core energies $\Delta U$, introducing them as the internal interaction energy of the components, constituting the core

$$\Delta U_{\text{core}} = \frac{1}{2} \left[ \sum_{i \neq j} q_i q_j \Phi(r_{ij}) \right]_{\text{core}}.$$ (22)

The sum is running over all the interacting pairs of the core particles. The mean interaction energies obtained this way in simulations and estimated from the experimental data are collected in table 2.

If stable under external loading (in this case under thermal stress), the dislocation clusters show the same deformation features as any elastic body. Then the interaction of the dislocations constituting the cluster can be studied by measuring the occurrence (probability) of the core configurations [16, 17]. For instance, the histograms of the core diagonals of the compact clusters shown in figures 11 and 12 provide the core geometrical factor.

Dislocation clusters have a finite lifetime with respect to dissociation or annihilation, which is strongly dependent on the external conditions (see table 2). For instance, in our simulations a given cluster on average exists on the scale of a few Coulomb times at a relatively high temperature; see table 2. There are many processes responsible for disintegration. For instance, at a sufficiently strong external stress stretching even a stable cluster dissociates.
Figure 12. Compact clusters recovered from the experimental data obtained with a recrystallizing complex plasma [23, 24]. The panels show the histograms of the core diagonals computed (a) at a high temperature (table 2, case 3) and (b) at a low temperature (table 2, case 2). On average, the core structure is eventually universal, practically independent of the temperature.

One more striking symmetry feature, related to dissociation, is interesting to mention. As in the case of the cluster structural asymmetry considered in section 5 (see figure 3), the simulations, and likewise the observations, demonstrate an interesting peculiarity revealing an escape asymmetry of newly born free dislocations. This process resembles discrete symmetry breaking for the following reason: whatever the orientation of the cluster as a whole, escaping dislocations can glide only along two crystallographic directions (along Burgers vectors). This naturally explains the asymmetry of the escape directions and the chirality of the defect configurations revealed by the newly nucleated dislocations in experiments [51]. In other words, the hexagonal symmetry is broken by the direction of dissociation of a single pair, which is arbitrary.

7. Conclusion

The collection of point defects in 2D plasma crystals, which we have exhibited, consists of interstitials, vacancies and compact dislocation clusters, resembling those observed and/or simulated in colloids. Still, new elements are to be included in the list—for instance, the mobile interstitials mediated by the focused collisions, traveling along the closest-packing lattice rows.

We have applied molecular dynamics simulations to study the dynamics of the point defects and defect clusters in a 2D plasma crystal sustaining the charged micro-particles confined to two dimensions and interacting mutually through a screened Coulomb (Yukawa) central potential. This allowed us to study in detail the nucleation of dislocations, vacancies, interstitials and compact dislocation clusters, and particularly to demonstrate the energy balance during nucleation. We estimated the work of nucleation, and showed that this work is approximately...
equally divided among friction energy loss and configuration energy. Friction, hence, must not be ignored in the balance even if our system is not overdamped. The second important point is the equipartition of the energy component (potential and kinetic) variations. Taking into account that plasma crystals are highly non-ideal, it is a rather surprising fact. This is fine balance is indeed controlled by the virial variation.

Some properties of the defect clusters look distinctively different from those observed in colloids. Our simulations and experiments showed that the dislocation clusters associated with point defects in plasma crystals happened to be relatively more compact structures. This is a very important message: most of the deformation involved is concentrated in the close proximity of the point defect. Substantially, the compactness of the defect clusters is a benefit of plasma crystals. On the other hand (‘every medal has two sides’), since most of the deformation is in the near-field region, it is a challenge to adequately introduce an elastic neighborhood, commonly associating with a point defect. The reason for the more compact structure of the dislocation clusters is the presence of an external confinement, which enables the formation of a stable system of negatively charged particles in complex plasmas. It is worth addressing this feature in more detail in future investigations.

The simulations show that either strain-induced or the thermally activated nucleation of the dislocations in plasma crystals starts from the formation of (meta-stable) compact dislocation clusters. We estimated the activation energy, which happened to be in fairly good agreement with observations. Using data from the simulations and experiments, we studied the statistical characteristics of the defects in the plasma crystal. This helped to explore and quantify the topology and energetics of the simplest dislocation clusters. Both in simulations and experiments, the compact dislocation cluster ($5^7$-associations of the fivefold and sevenfold coordinated particles) happened to be as frequent as, e.g., dumbbell interstitials ($7^5$-associations of the fivefold and sevenfold coordinated particles), and have approximately the same lifetime (see table 2). It is worth noting that the results obtained from numerical simulations describe the dislocation nucleation observed recently in experiments fairly well.

It is common knowledge that the point defects play an important part in defining many aspects of the structural and dynamical properties of crystals. Many important features of the spatial structure of crystals can be modeled with the help of plasma crystals, which are perfectly suited to study the symmetry and multi-scale plasticity of a 2D lattice layer.

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