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Extended topological defects as sources and outlets of dislocations in spherical hexagonal crystals

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Extended topological defects (ETDs) arising in spherical hexagonal crystals due to their curvature are considered. These prevalent defects carry a unit total topological charge and are surrounded by scalene pentagonal boundaries. Topological peculiarities of reactions between ETDs and dislocations are considered. Similarly to boundaries of the usual planar crystalline order the ETDs emit and absorb the dislocations without preservation of their dislocational charge. Dislocations located inside the ETD area lose it and the enforced ETD decay can proceed in different ways without conservation of the total Burgers vector of the dislocations emitted.

Two-dimensional (2D) ordered structures with an unusual topology are under discussion since the very beginning of the 20th century. Trying to explain the periodic law of Mendeleev, J.J. Thomson proposed a model of atom, according to which the electrons confined at the sphere surface interact by means of Coulomb potential. Determination of the equilibrium position of repelling equally-charged particles on the sphere was called the Thomson problem [1]. Later, it was generalized to the case of non-Coulomb potentials [2]. Tammes considered the similar problem how N identical spherical caps should be packed on the sphere to provide the maximal cap size [3].

Experimental investigation of the behavior of colloidal particles located at the interface between two liquids was started by Ramsden [4] in 1903. More than a century later this study led to the synthesis of nanoporous capsules – colloidosoms [5]. Similar ordered structures appear in various systems. For example, they are formed by viral capsid proteins [6,7], localized electrons in multi-electron bubbles in superfluid helium [8], Pickering emulsion on spherical surfaces [9–11] and even occur in coding theory [12,13]. All these natural and synthetic objects are more or less ordered structures forming the 2D closed shells topologically equivalent to a sphere.

Due to the curved topology new crystallographic peculiarities appear in these systems [14]. One of such peculiarities is the inevitable existence of topological defects that causes the curvature of the ordered 2D spherical structures. Depending on presence of the other types of defects the spherical structures can be divided into two groups. The viral capsids from the first group demonstrate the 'perfect' spherical crystalline [6] or quasicrystalline [15] structures with the regular curvature-related topological defects only. The spherical crystals from the second group are more disordered. Examples are solid colloidosomes and 2D colloidal crystals formed on the spherical surfaces [5,9,11]. The important features of these systems are presence of dislocations usual for the planar hexagonal lattice and not so symmetric arrangement of topological defects, which often take the form of scars [10]. The other 'exotic' ETDs unconventional for the planar geometry are also possible. The related defect motifs were studied in the frame of the Thomson problem [16,17]. Recently, formation of ETDs with a square order inside on the colloidosome surface [5], was explained [18] in the frame of Lennard-Jones inter-particle coupling.

The pioneer experimental work [10] devoted to the peculiarities of the spherical order in colloidal crystals was published a decade ago. It was found that this order is very sensitive to the ratio R/a, where R is the radius of the sphere and a is an average particle radius. For $R/a \geqslant 5$ the authors of Ref. [10] have found linear defects, which they called grain boundaries, or scars. These defects present the chains consisting of closely located particles with different surroundings. Particles having 5 or 7 nearest neighbors sequentially alternate in the scars, while the other particles have 6 neighbors. Therefore the scar is usually treated as a sequence of elementary 5-fold and 7-fold disclinations. These defects

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have been investigated in subsequent experimental and theoretical studies [11,19]. The theory [19] successfully considers the spherical hexagonal order in colloidal crystals as a result of simple repulsion of particles retained on a spherical surface and explains formation of scars in the frames of continuum approach. However, as demonstrated below for the case of the simplest repulsive pair potentials, the emerging spherical hexagonal order is essentially distorted in the relatively wide areas of ETDs, where only the Delaunay triangulation [20] can match the nodes with their neighbors and thus localize the relatively narrow scars.

The aim of this Letter is to demonstrate new topological properties of ETDs arising in spherical crystals due to their curvature. Here we show that: (i) enforced decay of the ETD does not conserve the total Burgers vector of the dislocations emitted; (ii) dislocations within the ETD area lose their dislocational charge and the order outside the defect doesn't display their existence in any way.

We start our consideration from some more or less known peculiarities of spherical hexagonal order. Let us recall that the self-assembly of 2D structure on a non-planar surface can be described by the conditional minimization of the system free energy F with respect to coordinates of the system particles. The condition imposed is that any particle during minimization should be on the surface under consideration. The order in the spherical colloidal crystals is successfully modeled and analytically studied in the frame of the simplest power low pair potentials [16,17,19] when the free energy has the form:

$$F = \varepsilon \sum_{j>i}^{N} \frac{1}{r_{ij}^{\alpha}}, \tag{1}$$

where r_{ij} is the distance between ith and jth particles, N is the number of particles. The exponent $\alpha = 1$ for Coulombic long range interaction of charges, while the solution of Tammes problem [3] (very short-range interaction) corresponds to $\alpha \to \infty$. The interaction of particles by means of Lennard-Jones pair potential is also reduced to energy (1) with $\alpha = 12$ provided the particles on a sphere are located closely enough and the term associated with their repulsion prevails over their attraction. Note also that the conditional minimization of Eq. (1) yields different equilibrium structures corresponding to the same values of N and α depending on the initial distribution of particles.

Numerically obtained spherical structure with $N = 700$ particle and $\alpha = 12$ (see Fig. 1) is a typical one for the N range from 400 to 1000 and for the α values in the range of several tens (for larger α the numerical minimization of (1) becomes difficult). Analogous structures corresponding to minima of energy (1) can be also obtained with the help of public domain programs, see for example [21]. Global-minima spherical structures with $\alpha = 1$ are extensively studied. The putative list of them for $N < 20\,000$ can be found at the same site, see also [17]. The hexagonal order in the global-minima structures is more perfect than in the local-minima ones and the areas occupied by the extended defects are smaller. However, for the same N value the equilibrium energies of global and local-minima structures are very close [14]. If this value increases, the difference between the equilibrium energies is reduced and the number of hexagonal structures with the similar energies, but different arrangement of particles in defects, grows exponentially [22]. Due to this fact, it is much more probable to observe experimentally a colloidal crystal corresponding to one of numerous local minima than that with the globally minimal free energy. This point of view is also supported by our observation that ETDs in experimental colloidal crystals [5,10,11] are more complicated (for example, the scars are longer) than the defects in the global-minima theoretical spherical structures presented in [21].

Note that the total topological charge [10] of the ETD is completely determined by the number of sides of characteristic poly-

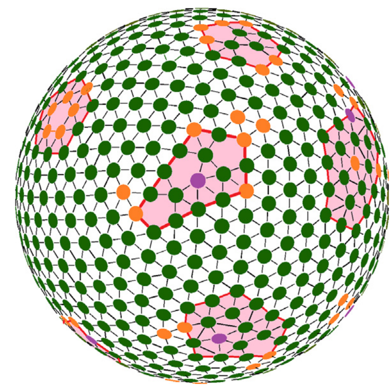

Fig. 1. (Color online.) Spherical structure with $N = 700$ particles. Extended topological defects with the unit positive topological charge are highlighted by red pentagons. Orange and purple circles denote particles with the smallest ($E_p < 0.5E_{avg}$) and the largest ($E_p > 1.34E_{avg}$) energy per particle, respectively. Here E_p is the energy per particle and E_{avg} is the average energy per particle.

gon, surrounding the defect provided the polygon satisfies two following conditions: (1) the polygon sides pass only through the nodes with six neighbors; (2) the angle between the nearest polygon sides in the initial planar hexagonal order is equal to $2\pi/3$. Then the total topological charge q of the defect is simply defined as

$$q = 6 - m, \tag{2}$$

where m is the number of sides of the characteristic polygon. The conventional dislocations without a topological charge can always be surrounded by hexagons. The ETDs with the total charge $q = 1$ are surrounded by pentagons which are scalene in general case. Let us recall that the simplest local 5-fold disclination (surrounded by the regular pentagon) is usually associated with elimination of the $\pi/3$ sector from the hexagonal planar lattice [14]. In general, the edges of the eliminated sector can be glued after some relative shift equal to a translation of the initial hexagonal order. Such a shift implies that the characteristic pentagon is scalene and the initial hexagonal order near the top of the resulting solid angle is broken strongly within the defect area. But these peculiarities cannot change the total topological charge of the defect provided it is surrounded by the outer hexagonal order.

We have obtained about 50 spherical structures, with the number of ordered repulsive particles from 700 to 1000. Different initial random distributions of particles and different algorithms of energy (1) minimization (including the algorithm [23]) regularly resulted in appearance of extended areas with essentially distorted hexagonal order. In all the cases, the hexagonal order surrounding the defects was global. We have found no defects which do not allow the continuous circulation around. This particle arrangement corresponds always to more or less defective mapping of a single planar hexagonal lattice onto the sphere by means of the icosahedron net. We were always able to localize exactly twelve ETDs surrounded by pentagons. These defects repel each other and are located approximately near the vertices of an icosahedron (see Fig. 1). Spherical structures with arrangement of defects near the vertices of an icosahedron were obtained theoretically [19] and observed experimentally [11]. These topologically induced defects of spherical hexagonal order are usually treated as linear scars [10,11,19]. However, as we explain below such an interpretation of the defects is incomplete.

Let us recall, that the scars were initially defined as 'high-angle (30°) grain boundaries, which terminate freely within the crystal' [10]. Later it was understood that the scars have a variable rotation angle from 0° (at the scar ends) to 30° (at the scar center) [11]. Our numerical simulations demonstrate that inside the ETD area the structure is strongly disordered (see Figs. 1 and 2)