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PAIR INTERACTION OF COAXIAL CIRCULAR PRISMATIC DISLOCATION LOOPS IN ELASTIC SOLIDS WITH SPHERICAL SURFACES

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Abstract. In the present work, the pair interaction of coaxial circular prismatic dislocation loops (PDLs) arbitrary placed in elastic solids with free spherical surfaces is considered. The analytical solutions for the pair interaction energies of PDLs in an elastic sphere, an elastic medium with a spherical pore and a spherical layer are given in the form of double power series and illustrated by energy maps built in the space of the normalized PDL radii and axial positions. The results can be used for analyzing the theoretical models of stress relaxation processes in bulk and hollow core-shell nanoparticles and pentagonal particles, which occur through the formation of dislocation ensembles.

Keywords: prismatic dislocation loops, dislocation ensembles, stress relaxation

1. Introduction

Dislocation loops are typical defects in solids, which play a significant role in the physics and micromechanics of crystalline materials [1,2]. In particular, the formation of prismatic dislocation loops (PDLs) is one of the main mechanisms of elastic strain and stress relaxation in solid-state structures containing inhomogeneities and pores. For instance, the ensembles of concentric PDLs lying in the same plane and encircling the highly compressed precipitates in gadolinium gallium garnet crystals were examined by optical microscopy in [3,4]. Subsequently, this mechanism was theoretically described in [5] for the case of generation of a single PDL encircled spherical inclusion. The generation of a misfit PDL at the interface of the dilatational spherical inclusion was theoretically investigated in [6]. Another relaxation mechanism is the punching of ensembles of coaxial PDLs by the inclusion to the matrix. It was observed experimentally in [7-9] and then studied by analytical calculations [10] and dislocation dynamics computer simulations [11]. The generation of satellite PDLs as the effective relaxation mechanism in GaAs films containing As-Sb clusters subjected to one-dimensional dilatation eigenstrain was experimentally [12,13] and theoretically [14,15] investigated.

To analyze the critical conditions of PDL formation, the authors of the aforementioned theoretical models [5,6,10,14,15] used the well-known solution for the strain energy of a PDL in an infinite homogeneous elastic medium, given by Dundurs and Salamon [16], in which case the image force effects on the relaxation processes were neglected. This limitation could

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be overcome by using strict analytical solutions of relevant boundary-value problems in the theory of elasticity for PDLs in solids with spherical surfaces/interfaces.

By now, some strict analytical solutions describing the elastic fields and energies of circular PDLs in an infinite medium [16-18], near a flat free surface [19] and a planar interface [16,20], in thin plates [21,22], in homogeneous [23-25] and heterogenous core-shell [26] cylinders as well as in solids with spherical boundaries [27-31] have been fairly well discussed. The displacement field of a circular PDL in an elastic sphere was first presented in [27]. The elastic fields and energy of a circular PDL coaxial to the spherical pore in an infinite medium were obtained in [28] that allowed to analyze a critical condition for punching of a single PDL by the bubbles (pores under pressure) and verified these results with experimental observations of PDL ensembles in irradiated materials containing helium [32,33] or hydrogen [34] in bubbles. Recently, similar solution has been suggested to use in dislocation dynamics computer simulations [31]. The case of dislocation emission induced by the spherical pore under remote loading was also studied by molecular dynamics simulations [35,36].

The displacement field of a circular dislocation loop occupying an arbitrary position inside an elastically inhomogeneous core-shell spherical particle was found in [29]. The solution was given in the form of double series of vector functions with unknown coefficients which have to be determined by solving an infinite system of algebraic equations. The authors of [29] demonstrated their analytical results with a numerical calculation of the image force acting on a PDL symmetrically placed in the core that seems difficult to use in physical applications.

A more applicable solution, from our point of view, is presented in [30] where the stress field of a circular PDL is obtained in terms of the Legendre polynomials series for the following cases: an elastic sphere, an infinite elastic medium with a spherical pore, and an elastic spherical layer with free surfaces. The corresponding solutions have been applied for analyzing the initial stages of stress relaxation processes through the formation of individual PDLs in bulk [37] and hollow [38] core-shell nanoparticles, in icosahedral [39] and decahedral [40,41] small particles (see also a brief review [42]). These theoretical models give results which are in good agreement with experimental data [43,44].

Thus, the aforementioned strict analytical solutions have been used for analyzing the critical conditions of stress relaxation through generation of individual PDLs. However, both the experimental examinations and computer simulations show that, in many real structures, a number of similar PDLs can nucleate and behave in tight interaction with each other, which requires the development of suitable mathematical means for studying these situations. One of such means is the energy of pair interactions between PDLs.

In the present work, we consider the interaction of two coaxial circular PDLs arbitrary placed in different elastic bodies with free spherical surfaces such as an elastic sphere, an elastic medium with a spherical pore, and a spherical layer. Using the strict analytical solution of the boundary-value problem for a circular PDL in an elastic sphere [30], we find an analytical form for the interaction energy and illustrate this result by energy maps built in the space of the normalized PDL radii and axial positions. In our further work, we are going to use these results in analyzing theoretical models of stress relaxation processes in core-shell nanoparticles and pentagonal particles, which occur through the formation of various dislocation ensembles.

2. Model

Consider an elastically isotropic spherical layer with inner and outer radii a_p and a, respectively, containing a pair of interstitials (for definiteness) circular PDLs which are characterized by the following plastic distortion component [45]:

$$\beta_{zz}^{(k)} = b_k H(1 - r/c_k)\delta(z - z_k), \quad k = 1, 2, \tag{1}$$

where b_k is the Burgers vector magnitude of the PDL-k, $H(t)$ is the Heaviside function, $\delta(z-z_k)$ is the Dirac delta function, c_k is the radius of the PDL-k, and z_k is its coordinate (see Fig. 1).

The interaction energy W_{int}^{1-2} between PDL-1 and PDL-2 in the spherical layer can be determined as the work spent to create the PDL-1 in the stress field $\sigma_{zz}^{(2)}$ of the PDL-2:

$$W_{int}^{1-2} = \int_V \beta_{zz}^{(1)}\sigma_{zz}^{(2)} dV = b_1 \int_V H(1 - r/c_1)\delta(z - z_1)\sigma_{zz}^{(2)} dV = b_1 \int_{S_1} \sigma_{zz}^{(2)}\Big|_{z=z_1} dS = 2\pi b_1 \int_{\xi}^{c_1} \sigma_{zz}^{(2)} r dr, \tag{2}$$

where r is the polar radius; $\xi = 0$ in the case when the PDL-1 plane does not intersect the inner spherical surface, i.e. when $z_1 \geq a_p$, and $\xi = \sqrt{a_p^2 - z_1^2}$ in the case when the PDL-1 plane intersects the inner spherical surface, i.e. when $z_1 < a_p$.

According to [30], the axial stress $\sigma_{zz}^{(2)}$ of PDL-2 in the elastic layer can be presented as a sum of the axial stress ${}^{\infty}\sigma_{zz}^{(2)}$ of PDL-2 in an infinite elastic medium and an additional term ${}^{*}\sigma_{zz}^{(2)}$ which provides the fulfillment of the boundary conditions on the free spherical surfaces:

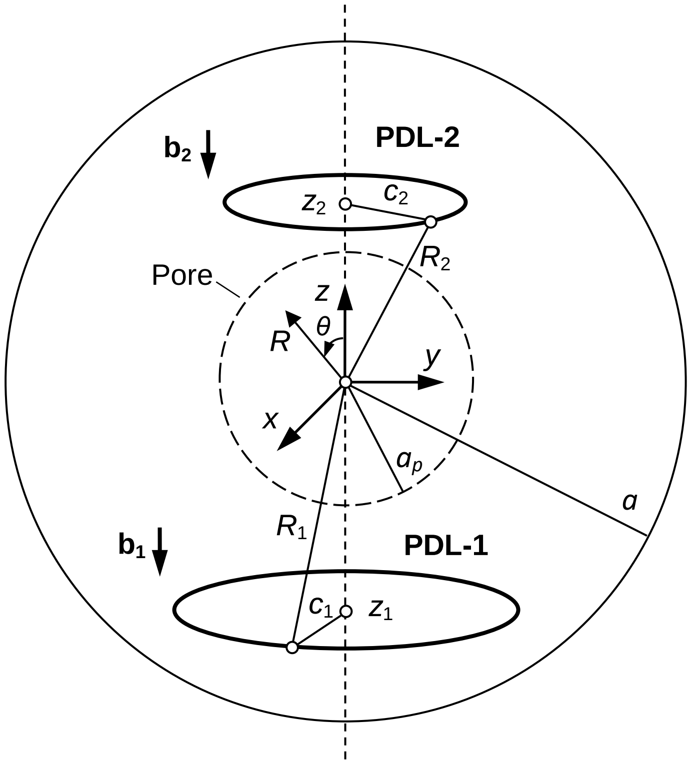

Fig. 1. A pair of interstitial circular PDLs in a spherical layer. The corresponding coordinate system is located in the center of spherical surfaces

$$\sigma_{zz}^{(2)} = {}^{\infty}\sigma_{zz}^{(2)} + {}^{*}\sigma_{zz}^{(2)}, \tag{3a}$$

$${}^{\infty}\sigma_{zz}^{(2)} = -\frac{Gb_2}{2(1-\nu)}\left[\frac{1}{c_2} J(1,0;1) + \frac{|z - z_2|}{c_2^2} J(1,0;2)\right], \tag{3b}$$

$${}^{*}\sigma_{zz}^{(2)} = \sigma_{RR}\cos^2\theta + \sigma_{\theta\theta}\sin^2\theta - \sigma_{R\theta}\sin 2\theta, \tag{3c}$$

$$^{*}\sigma_{RR}^{(2)}=2G\sum_{n=0}^{+\infty}\left[-A_n^{(2)}(n+1)(n^2-k-2-2\nu)R^n-B_n^{(2)}n(n-1)R^{n-2}+\right.$$
$$\left.+\frac{C_n^{(2)}n}{R^{n+1}}(n^2+3n-2\nu)-\frac{D_n^{(2)}}{R^{n+3}}(n+1)(n+2)\right]P_n\,(\cos\theta)\,, \tag{3d}$$

$$^{*}\sigma_{R\theta}^{(2)}=2G\sum_{n=1}^{+\infty}\left[-A_n^{(2)}(n^2+2\,n-1+2\nu)R^k-B_k^{(2)}(n-1)R^{n-2}-\right.$$
$$\left.-\frac{C_n^{(2)}}{R^{n+1}}(n^2-2+2\nu)+\frac{D_n^{(2)}}{R^{n+3}}(n+2)\right]\frac{dP_n\,(\cos\theta)}{d\theta}\,, \tag{3e}$$

$$^{*}\sigma_{\theta\theta}^{(2)}=2G\sum_{k=0}^{+\infty}\left\{\left[-A_n^{(2)}(n+1)(n^2+4n+2+2\nu)R^n-B_n^{(2)}n^2R^{n-2}+\right.\right.$$
$$\left.+\frac{C_n^{(2)}n}{R^{n+1}}(n^2-2n-1+2\nu)-\frac{D_n^{(2)}(n+1)^2}{R^{n+3}}\right]P_n\,(\cos\theta)-$$
$$-\left[A_n^{(2)}(n+5-4\nu)R^n+B_n^{(2)}R^{n-2}+\frac{C_n^{(2)}}{R^{n+1}}(-n+4-4\nu)+\frac{D_n^{(2)}}{R^{n+3}}\right]\frac{dP_n(\cos\theta)}{d\theta}\cot\theta\,, \tag{3f}$$

where G is the shear modulus, ν is the Poisson ratio, $J(m,n;p)$ are the Lipchitz-Hankel integrals defined as $J\left(m,n;p\right)=\int_0^\infty J_m(\kappa)J_n(\kappa\,r\,/\,c_2)\exp[-\kappa\,|\,z-z_2\,|\,/c_2]\kappa^p d\kappa$, $J_m(\kappa)$ and $J_n(\kappa\,r/c_2)$ are the Bessel functions, $A_n^{(2)}$, $B_n^{(2)}$, $C_n^{(2)}$, and $D_n^{(2)}$ are the coefficients determined in [30] from the boundary conditions on the free inner and outer spherical surfaces, and $P_n(t)$ are the Legendre polynomials determined by the following explicit formula

$$P_n(t)=\frac{1}{2^n}\sum_{s=0}^{[n/2]}(-1)^s\binom{n}{s}\binom{2n-2s}{n}t^{n-2s}\,. \tag{4}$$

Here $t=\cos\theta$, $[n\,/\,2]$ gives the greatest integer less than or equal to $n\,/\,2$, and $\binom{n}{s}$ are the binomial coefficients.

Substituting (3a) to (2), we obtain after integration

$$^{\infty}W^{1-2}=\frac{\pi Gb_1b_2}{(1-\nu)}\left[r\,J(1,1;0)+\frac{|\,z-z_2\,|}{c_2}rJ(1,1;1)\right]_{r\,=\,\xi}^{r\,=\,c_1}\Bigg|_{z\,=\,z_1}\,. \tag{5}$$

Then one can simplify equations (3c-f) for $^{*}\sigma_{zz}^{(2)}$ by using the following recurrence relations for the Legendre polynomials [30]:

$$t^2P_n\,(t)=\frac{(n+1)(n+2)}{(2n+1)(2n+3)}P_{n+2}(t)+\frac{2n^2+2n-1}{(2n-1)(2n+3)}P_n(t)+\frac{n(n-1)}{(2n-1)(2n+1)}P_{n-2}(t)\,, \tag{6a}$$

$$t\sqrt{1-t^2}\,P_n^1(t)=\frac{n(n+1)(n+2)}{(2n+1)(2n+3)}P_{n+2}(t)-\frac{n(n+1)}{(2n-1)(2n+3)}P_n(t)-\frac{(n-1)n(n+1)}{(2n-1)(2n+1)}P_{n-2}(t)\,, \tag{6b}$$

where $P_n^1(t)=-\sqrt{1-t^2}\,dP_n\,(t)\,/\,dt$.

Substituting recurrence relations (6) to (3c), after some algebra we finally find

$$^{*}\sigma_{zz}^{(2)}=\frac{Gb}{1-\nu}\sum_{n=0}^{+\infty}\left[A_n^{(2)}\,\frac{2(n+1)(1+\nu-2n\nu-2n^2)}{2n-1}R^n+B_{n+2}^{(2)}(n+1)(n+2)R^n\right.$$
$$+A_{n+2}^{(2)}\frac{(n+2)(n+3)(2n^2+9n+7)}{2n+3}R^{n+2}-\frac{2n(1-3\nu+2n(2-\nu)+2n^2)}{2n+3}\frac{C_n^{(2)}}{R^{n+1}}+$$

$$+(n-1)n\frac{D_{n-2}^{(2)}}{R^{n+1}}-\frac{(n-2)n(2n^2-7n+5)}{2n-1}\frac{C_{n-2}^{(2)}}{R^{n-1}}\Bigg]P_n\,(\cos\theta)\,, \tag{7}$$

where $C_{-2}^{(2)}=D_{-2}^{(2)}=C_{-1}^{(2)}=D_{-1}^{(2)}=0$.

With Eq. (7) and taking into account that, for $z = z_1$, the relations $\cos\theta = z_1 / R$ and $r\,dr = R\,dR$ hold, integral (2) gives

$$\begin{aligned}{}^{*}W^{1-2}=\frac{\pi G b_1 b_2}{1-\nu}\sum_{n=0}^{+\infty}\Bigg[&A_n^{(2)}\frac{2(n+1)(1+\nu-2n\nu-2n^2)}{2n-1}Q_{n,1}+B_{n+2}^{(2)}(n+1)(n+2)Q_{n,1}\\&+A_{n+2}^{(2)}\frac{(n+2)(n+3)(2n^2+9n+7)}{2n+3}Q_{n,2}-C_n^{(2)}\frac{2n(1-3\nu+2n(2-\nu)+2n^2)}{2n+3}T_{n,1}+\\&+D_{n-2}^{(2)}(n-1)nT_{n,3}-C_{n-2}^{(2)}\frac{(n-2)n(2n^2-7n+5)}{2n-1}T_{n,3}\Bigg],\end{aligned} \tag{8}$$

where $Q_{n,l}$ and $T_{n,l}$ are polynomials determined by equations

$$Q_{n,l}=\sum_{s=0}^{[n/2]}\frac{(-1)^s}{2^n(s+l)}\binom{n}{s}\binom{2n-2s}{n}z_1^{n-2s}\left(R_1^{2(s+l)}-\zeta^{2(s+l)}\right), \tag{9a}$$

$$T_{n,l}=\sum_{s=0}^{[n/2]}\frac{(-1)^s}{2^n(-2k+2s+l)}\binom{n}{s}\binom{2n-2s}{n}z_1^{n-2s}\left(R_1^{-2k+2s+l}-\zeta^{-2k+2s+l}\right). \tag{9b}$$

Here $\zeta = z_1$ if $z_1 \geq a_p$, and $\zeta = a_p$ if $z_1 < a_p$.

Thus, the interaction energy W_{int}^{1-2} for PDL-1 and PDL-2 in the spherical layer is given by

$$W_{int}^{1-2}={}^{\infty}W^{1-2}+{}^{*}W^{1-2}\,, \tag{10}$$

where ${}^{\infty}W^{1-2}$ is determined by Eq. (5) and ${}^{*}W^{1-2}$ by Eqs. (8) and (9).

3. Results

To illustrate the results obtained, consider an example of the pair interaction between PDL-1, which has arbitrary radius c_1 and axial position z_1, and PDL-2 with fixed radius $c_2 = 100b_2$ and axial position $z_2 = 0$. Figures 2a-d show the maps of the interaction energy W_{int}^{1-2} in normalized coordinates of radius c_1/c_2 and axial position z_1/c_2 of PDL-1 in (a) an infinite medium, (b) an elastic sphere of radius $a = 1.5c_2$, (c) an infinite medium with a spherical pore of radius $a_p = 0.5c_2$, and (d) a spherical layer of radii $a_p = 0.5c_2$ and $a = 1.5c_2$. As is seen, the interaction energy of PDLs strongly depends on their radii and positions in the elastic body. Moreover, it is highly sensitive to the presence of the inner and outer free surface in the case when at least one of the PDLs is localized near the surface. It is worth noting that, in this case, the outer free surface makes a greater effect on the interaction energy than the inner free surface. The most evident and interesting manifestation of the outer surface effect is the region of negative values of the interaction energy near the equator and the outer free surface (at the right bottom corner of the maps in Figs. 2(b,d). It means that PDL-1 of radius $0.9a < c_1 < a$ is attracted to immobilized PDL-2 in this region, while in all the remaining area of the body, where the interaction energy is positive, PDL-1 is repulsed of PDL-2. In contrast, the inner free surface does not give such effect.

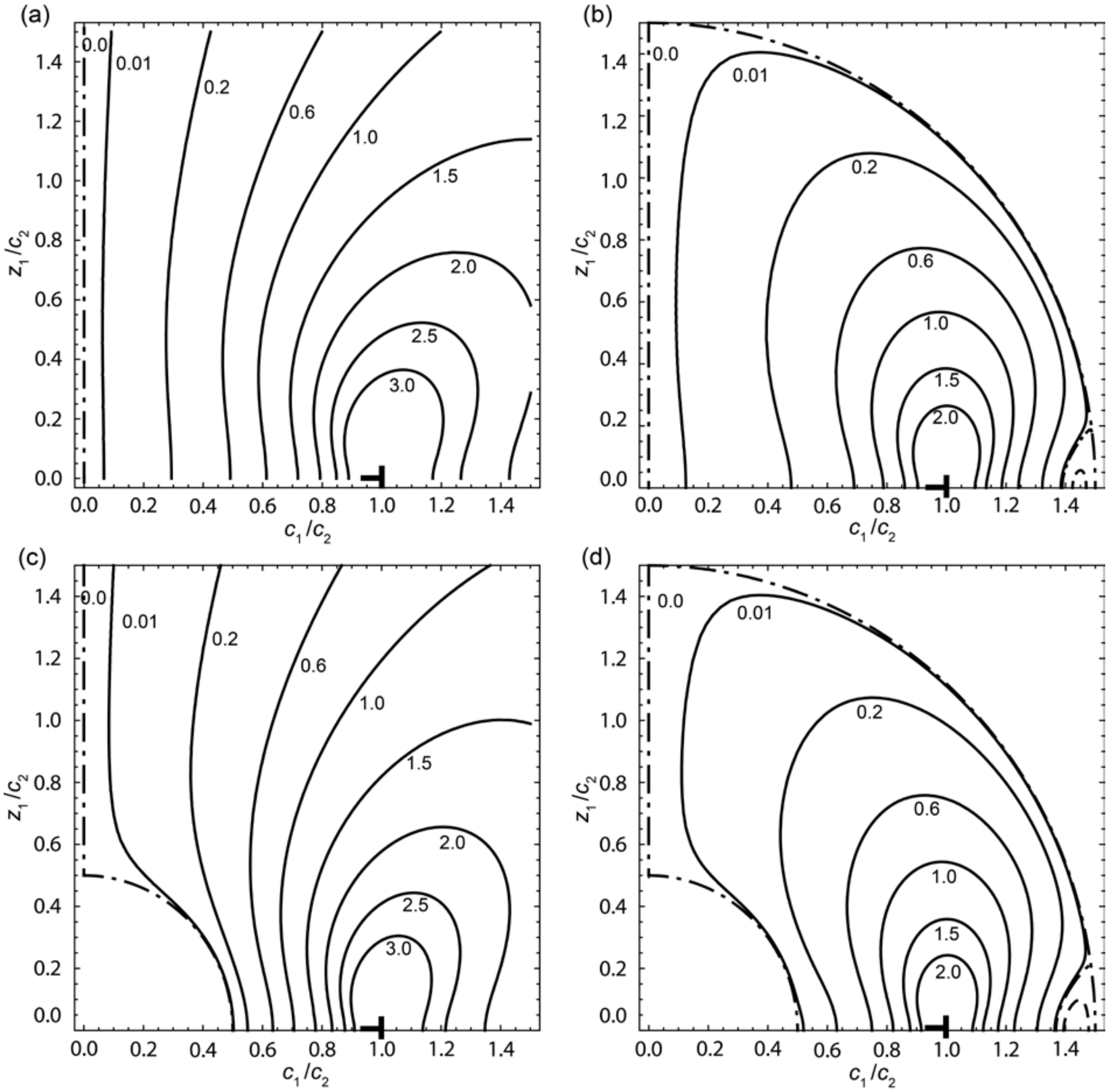

Fig. 2. The maps of pair interaction energy W_{int}^{1-2} for PDL-1 with arbitrary radius c_1 and position z_1 and PDL-2 of radius $c_2 = 100b_2$, placed in plane $z_2 = 0$ in (a) an infinite medium, (b) an elastic sphere of radius $a = 1.5c_2$, (c) an infinite medium with a spherical pore of radius $a_p = 0.5c_2$, and (d) a spherical layer of radii $a_p = 0.5c_2$ and $a = 1.5c_2$.
The energy is given in units $Gb_1b_2c_2$

4. Conclusions

The phenomenon of pair interaction of circular PDLs in solids with spherical boundaries such as an elastic sphere, an infinite medium with a spherical pore, and a spherical layer with free surfaces is studied in detail. An explicit formula for interaction energy of two coaxial circular PDLs is obtained in the form of double power series. This result is illustrated by maps of the interaction energy in the space of PDL radii and axial positions. It is shown that the interaction energy of PDLs is strongly screened by free spherical surfaces when at least one of the PDLs is localized near the surface. The outer free surface makes a greater effect on the interaction energy than the inner free surface. In particular, there is a region near the equator and the outer free surface, where the interaction energy changes its sign. The inner free surface does not give such effect. Our results give an opportunity to analyze stress relaxation processes through the generation of PDL ensembles in porous materials as well as bulk and hollow core-shell nanoparticles and pentagonal particles.

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