

## DEFECTS, DISLOCATIONS, AND PHYSICS OF STRENGTH

# On Mechanical Characteristics of Nanocrystals

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**Abstract**—The dependence of the elastic moduli of a nanocrystal on its size is investigated theoretically with reference to a two-dimensional single-crystal strip. It is shown that the uncertainty (of a fundamental nature) in the size of a nanocrystal causes the determination of many of its mechanical characteristics to be ambiguous. It is found that the Cauchy–Green relations are modified and the elastic-constant tensor ceases to be symmetric; the size and shape of a nanocrystal render its mechanical properties more anisotropic. For a single-crystal strip, the Poisson ratio decreases and the Young modulus increases with decreasing thickness of the strip; in the case of a very thin crystal film (two atomic layers thick), these elastic moduli can differ from their macroscopic values by a factor of two. The size effects which make the continuum elasticity theory inapplicable to nanocrystals are estimated. The size effects that occur when the molecular dynamics method is applied for modeling macroscopic objects are also discussed. © 2002 MAIK “Nauka/Interperiodica”.

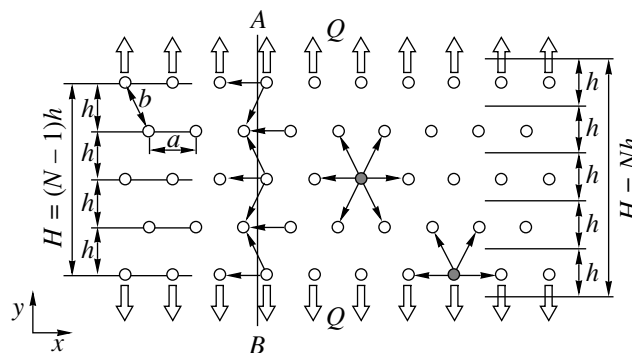
## 1. INTRODUCTION

The recent rapid development of nanotechnologies has generated a need for analytical models that can adequately describe the physical-mechanical properties of nanometer-sized objects. In most existing models, the main mechanical characteristics of nanocrystals are assumed to be identical to those measured for macroscopic crystals. However, when a structure consists of only a few atomic layers, discordance between its evident discreteness and the continuum models applied for describing the structure should manifest itself. The discrepancy between the values of the elastic moduli measured for microscopic and macroscopic samples has been pointed out by many investigators [1–3]. Unfortunately, direct measurements of the elastic characteristics of a nanometer-sized object are impossible; one is forced to use indirect methods [2, 4, 5]. One of the methods used for determining the elastic characteristics of such objects is the study of the microrelief that forms when a sample covered with an ultrathin film is stretched [2, 5, 6]. By solving the corresponding continuum problem on the stability of the thin-walled construction, one can determine the Poisson ratio and the Young modulus of the covering film from such experiments [1, 6, 7]. However, the values of the elastic characteristics determined in this way differ essentially from the corresponding macroscopic values. This discrepancy may be due to both the specific internal structure of the sputtered film and the discreteness of the film on a nanometer scale. This paper is devoted to studying the influence of the discreteness of a film on its elastic moduli and is a continuation of the study performed in [8].

To investigate the size effect for the mechanical characteristics of a material, we take, as a model, a two-dimensional strip of a single crystal with hexagonal closely packed (hcp) structure (triangle lattice). The atoms are assumed to interact via a pairwise potential. The main results are obtained by including only the nearest neighbor interaction; the effect of more distant neighbor atoms is estimated in Section 4. In determining the elastic moduli, we restrict our consideration to the case of tension and compression of a single crystal; the case of shear strain is not discussed in this paper.

## 2. DETERMINATION OF ELASTIC MODULI

We consider a two-dimensional single crystal (Fig. 1) infinitely long (along the  $x$  axis) and  $N \geq 2$  atomic layers thick (along the  $y$  axis). Each atom interacts only with nearest neighbor atoms, as shown in



**Fig. 1.** Model under study: two-dimensional single-crystal strip (schematic).

Fig. 1. Constant tensile forces  $Q$  are applied to the atoms situated at the ends of the crystal. The deformed state of the crystal is fully determined by the distance  $a$  between neighboring atoms in each layer and the distance  $h$  between adjacent layers. The distance between the nearest neighbor atoms belonging to adjacent layers is  $b$  (Fig. 1). Obviously, we have  $b^2 = a^2/4 + h^2$ . In the undeformed state, the lattice consists of equilateral triangles with sides  $a = b = a_0$  and the load applied to the ends is zero ( $Q = 0$ ). Let  $F(r)$  be the interaction force between two atoms separated by a distance  $r$  (the attractive force is considered to be positive). Then, the equilibrium condition (along the  $y$  axis) for an atom situated at the crystal surface has the form

$$Q = 2\frac{h}{b}F(b) \longrightarrow \sigma_2 \stackrel{\text{def}}{=} \frac{Q}{a} = 2\frac{h}{ab}F(b). \quad (1)$$

Here,  $\sigma_2$  is the normal stress applied along the  $y$  axis. Let us mentally cut the crystal along the vertical straight line AB (Fig. 1). The total normal force exerted on one part of the crystal by the other is

$$H\sigma_1 = NF(a) + (N-1)\frac{a}{2b}F(b). \quad (2)$$

Here,  $\sigma_1$  is the normal stress applied along the  $x$  axis; and  $H$  is the crystal thickness (along the  $y$  axis). The value of  $H$  cannot be determined unambiguously. For example, if the thickness is defined as the spacing between the layers lying at opposite ends of the crystal (Fig. 1), then  $H = (N-1)h$ . On the other hand, it is reasonable to define the crystal thickness as the product of the thickness of one layer multiplied by the number of layers, which gives  $H = Nh$ . For this reason, we define the thickness as

$$H \stackrel{\text{def}}{=} N_*h, \quad N-1 \leq N_* \leq N, \quad (3)$$

where the quantity  $N_*$  reflects the ambiguity of the definition of  $H$ . Since the strains are small, the forces acting in the crystal can be approximately written in the form

$$F(a) = C\Delta a, \quad F(b) = C\Delta b, \quad C \stackrel{\text{def}}{=} F'(a_0) > 0, \quad (4)$$

where  $C$  is the atomic-bond stiffness and the symbol  $\Delta$  indicates the deviation of a quantity from its corresponding value for an undeformed crystal. Let us denote the strains of the crystal along the  $x$  and  $y$  axes by  $\varepsilon_1$  and  $\varepsilon_2$ , respectively. We have

$$\varepsilon_1 \stackrel{\text{def}}{=} \Delta a/a_0, \quad \varepsilon_2 \stackrel{\text{def}}{=} \Delta h/h_0, \quad h_0 \stackrel{\text{def}}{=} \sqrt{3}a_0/2. \quad (5)$$

Substituting Eqs. (3)–(5) into Eqs. (1) and (2) yields the elasticity relations

$$\sigma_1 = C_{11}\varepsilon_1 + C_{12}\varepsilon_2, \quad \sigma_2 = C_{21}\varepsilon_1 + C_{22}\varepsilon_2, \quad (6)$$

where the stiffness coefficients  $C_{kn}$  are given by

$$C_{11} = \frac{3\sqrt{3}}{4} \frac{N-\frac{1}{9}}{N_*} C, \quad C_{12} = \frac{\sqrt{3}N-1}{4} \frac{C}{N_*}, \quad (7)$$

$$C_{21} = \frac{\sqrt{3}}{4} C, \quad C_{22} = \frac{3\sqrt{3}}{4} C.$$

It follows from Eq. (7) that the crystal under study is anisotropic. It will be recalled that an infinite two-dimensional hcp crystal is isotropic. Therefore, the anisotropy of the crystal under study is a size effect. Let us introduce the notation

$$v_1 \stackrel{\text{def}}{=} -\frac{\varepsilon_2}{\varepsilon_1} \Big|_{\sigma_2=0}, \quad E_1 \stackrel{\text{def}}{=} -\frac{\sigma_1}{\varepsilon_1} \Big|_{\sigma_2=0},$$

$$v_2 \stackrel{\text{def}}{=} -\frac{\varepsilon_1}{\varepsilon_2} \Big|_{\sigma_1=0}, \quad E_2 \stackrel{\text{def}}{=} -\frac{\sigma_2}{\varepsilon_2} \Big|_{\sigma_1=0}.$$

Here,  $v_1$  and  $E_1$  are the Poisson ratio and the Young modulus, respectively, characterizing the tension along the  $x$  axis and  $v_2$  and  $E_2$  are the respective quantities characterizing the tension along the  $y$  axis. Using Eqs. (6), we obtain

$$v_1 = \frac{C_{21}}{C_{22}}, \quad E_1 = C_{11} - v_1 C_{12} = \frac{D}{C_{22}},$$

$$v_2 = \frac{C_{12}}{C_{11}}, \quad E_2 = C_{22} - v_2 C_{21} = \frac{D}{C_{11}}, \quad (8)$$

$$D \stackrel{\text{def}}{=} C_{11}C_{22} - C_{12}C_{21}.$$

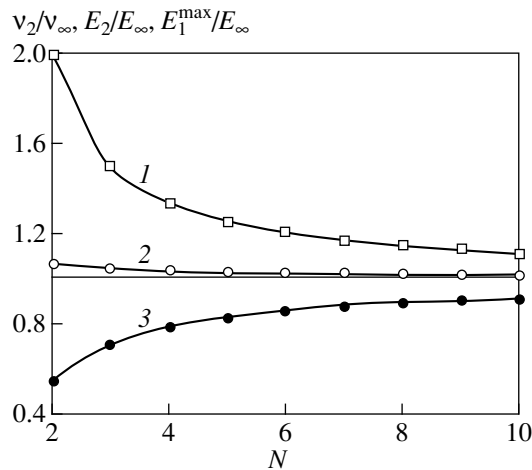
Substituting Eqs. (7) into Eqs. (8) yields the required expressions for the elastic moduli:

$$v_1 = v_\infty, \quad E_1 = \frac{N}{N_*} E_\infty,$$

$$v_2 = \frac{N-1}{N-\frac{1}{9}} v_\infty, \quad E_2 = \frac{N}{N-\frac{1}{9}} E_\infty. \quad (9)$$

Here,  $E_\infty = 2C/\sqrt{3}$  and  $v_\infty = 1/3$  are the values of the Young modulus and Poisson ratio corresponding to the infinite crystal, respectively [9, 10]. Let us discuss the formulas derived above.

When the crystal is stretched along the atomic layers, the Young modulus  $E_1$  essentially depends on the quantity  $N_*$ , i.e., on the definition of the thickness of the nanometer-sized crystal strip. If we put  $N_* = N$  (the maximum value of  $N_*$ ), then the Poisson ratio and Young modulus for tension along atomic layers will be independent of the number of layers. This is due to the fact that the crystal is infinite in the longitudinal direction. The Young modulus  $E_1^{\text{max}}$  corresponding to the



**Fig. 2.** Dependences of the Young modulus and Poisson ratio on the number of atomic layers. (1, 2) Young modulus in the longitudinal ( $E_1^{\max}/E_\infty$ ) and transverse ( $E_2/E_\infty$ ) directions, respectively, and (3) the relative Poisson ratio ( $v_2/v_\infty$ ) for stresses applied along the transverse direction.

minimum value  $N_* = N - 1$  is not a constant; it increases with decreasing number of atomic layers, so that at  $N = 2$ , this Young modulus becomes twice as large as  $E_\infty$  (Fig. 2). Therefore, the ambiguity of the definition of the Young modulus is essential in the case of small values of  $N$ .

When the crystal is stretched transversely to the atomic layers, both the Poisson ratio and the Young modulus vary with  $N$ ; namely, the Poisson ratio decreases and the Young modulus increases with decreasing number of layers (Fig. 2). It can be seen from Fig. 2 that the Poisson ratio  $v_2$  depends on  $N$  more heavily than does the Young modulus  $E_2$ . For example,

**Table 1.** Dependence of the elastic moduli of a nanocrystal on the number of atomic layers

$N$	$E_1^{\max}/E_\infty$	$v_2$	$v_2/v_\infty$	$E_2/E_\infty$
2	2.00	0.18	0.53	1.06
3	1.50	0.23	0.69	1.04
4	1.33	0.26	0.77	1.03
5	1.25	0.27	0.82	1.02
10	1.11	0.30	0.91	1.01
20	1.05	0.32	0.96	1.01
50	1.02	0.33	0.98	1.00
100	1.01	0.33	0.99	1.00

Note:  $E_1^{\max}$ ,  $E_2$ , and  $E_\infty$  are the Young moduli for a strip (in the longitudinal and transverse directions) and for an infinite crystal, respectively;  $v_2$  and  $v_\infty$  are the Poisson ratios for a strip (in the transverse direction) and an infinite crystal, respectively.

at  $N = 2$ , the deviation of the Young modulus from  $E_\infty$  does not exceed 6%, whereas the Poisson ratio in this case is nearly half as large as  $v_\infty$ .

As  $N \rightarrow \infty$ , the elastic moduli approach their values for an infinite crystal; these values do not depend on the direction of the applied stress. It should be noted that when the macroscopic values of the elastic moduli are used, the maximum relative error is roughly  $\frac{100\%}{N}$ .

For example, at  $N = 10$ , the deviation of  $E_1^{\max}$  and  $v_2$  from their respective macroscopic values is 11%, whereas at  $N = 100$ , this deviation is as small as 1% (Table 1).

### 3. STRAIN ENERGY

Let us discuss the elasticity relations (6). According to the macroscopic elasticity theory, the stresses  $\sigma_k$  and the elastic moduli  $C_{kn}$  are related to the specific strain energy through the Cauchy–Green equations

$$\sigma_k = \frac{\partial U}{\partial \varepsilon_k}, \quad C_{kn} \stackrel{\text{def}}{=} \frac{\partial \sigma_k}{\partial \varepsilon_n} = \frac{\partial^2 U}{\partial \varepsilon_k \partial \varepsilon_n}, \quad (10)$$

where  $U$  is the strain energy per unit volume. As before, we consider only the case of linear elasticity. From Eq. (10), it follows that  $C_{kn} = C_{nk}$ . Let us elucidate whether this relation holds for a nanocrystal. According to Eq. (7), we have

$$\frac{C_{12}}{C_{21}} = \frac{N-1}{N_*}. \quad (11)$$

Therefore, in the case of  $N_* = N$ , which is shown in Section 2 to be the most preferable, we have  $C_{12} \neq C_{21}$ . Does this result contradict the energy considerations? In order to clarify this issue, we consider the case where the crystal is stretched transversely to the atomic layers and find the change in the potential energy of a crystal domain with a fairly large length along the atomic layers. We have

$$dE_{\Pi} = N_x Q dy, \quad (12)$$

where  $E_{\Pi}$  is the total potential energy of the crystal,  $Q$  is the external force acting on an atom at the crystal surface (Fig. 1),  $dy$  is a small displacement of the upper surface of the crystal (the lower surface is assumed to be fixed), and  $N_x$  is the number of forces  $Q$  applied to the upper face of the crystal domain in question. We assume that  $N_x$  is sufficiently large for the size effects due to the finiteness of this domain to be negligible. The specific potential energy (per unit volume) is defined as

$$U \stackrel{\text{def}}{=} E_{\Pi} / (N_x a_0 N_* h_0). \quad (13)$$

The quantity in parentheses is the entire volume of the crystal domain, with  $N_x a_0$  being its dimension along the  $x$  axis and  $N_* h_0$  being the domain dimension (thick-

ness) along the  $y$  axis. As indicated in Section 2, the latter quantity cannot be determined unambiguously; this ambiguity also manifests itself in the definition of the specific internal energy. The quantities  $Q$  and  $dy$  are related to the stress and strain of the crystal through the equations

$$\begin{aligned} Q &= \sigma_2 a \approx \sigma_2 a_0, \\ dy &= (N-1)dh = (N-1)h_0 d\varepsilon_2. \end{aligned} \quad (14)$$

Substituting Eqs. (13) and (14) into Eq. (12) yields

$$\sigma_2 = \frac{N-1}{N_*} \frac{\partial U}{\partial \varepsilon_2}. \quad (15)$$

Thus, the macroscopic Cauchy–Green relations (10) do not hold in the case of finite values of  $N$ . Of course, Eq. (15) can be reduced to Eq. (10) by putting  $N_* = N-1$ . In this case, as follows from Eq. (11), the condition  $C_{12} = C_{21}$  is satisfied. However, it will be recalled that the Young modulus  $E_1$  essentially depends on  $N$  in this case, in contrast to the case of  $N_* = N$  [see Eq. (9)]. This situation also lends support to the fundamental conclusion that the size of a nanocrystal, as well as the quantities that depend on this size, can be defined differently. A definition appropriate in one case proves to be unsuitable in another. Thus, we find that the Cauchy–Green relations (10) in the case in question have to be modified as follows:

$$\sigma_1 = \frac{\partial U}{\partial \varepsilon_1}, \quad \sigma_2 = \frac{N-1}{N_*} \frac{\partial U}{\partial \varepsilon_2}, \quad C_{kn} = \frac{\partial \sigma_k}{\partial \varepsilon_n}. \quad (16)$$

The formula for  $\sigma_1$  in Eq. (16) is identical to that for a macroscopic crystal, because the crystal under study is infinite along the  $x$  axis.

Directly calculating the number of atomic bonds per unit length of the single-crystal strip, we find an explicit formula for the specific interaction energy  $U$ :

$$U = \frac{1}{N_* a_0 h_0} [N\Pi(a) + 2(N-1)\Pi(b)], \quad (17)$$

where  $\Pi(r)$  is the potential energy of interaction between two atoms separated by a distance  $r$ . The stiffness coefficients  $C_{kn}$  as calculated from Eqs. (16) with the specific energy given by Eq. (17) are identical to those calculated in Section 2 [see Eq. (7)].

#### 4. ALLOWANCE FOR INTERACTION WITH ATOMS OF THE SECOND COORDINATION SHELL

In the previous sections, we considered the interaction of an atom only with its nearest neighbor atoms (the first coordination shell). Including the interactions with more distant atoms highly complicates the calculation of the elastic moduli, because surface effects in this case distort the crystal lattice in the equilibrium state; these effects not only complicate the algebra but

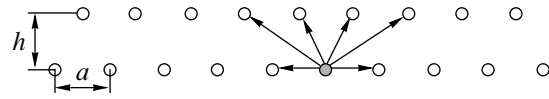


Fig. 3. Two-layered crystal (schematic).

also increase the ambiguity in defining the nanocrystal dimensions (because there is no certain lattice spacing). The latter circumstance, in turn, leads to an additional ambiguity in determining all quantities that depend on the nanocrystal size (such as the Young modulus). Another difficulty is associated with the fact that when the interaction with more distant atoms is included, the mechanical characteristics become strongly dependent on the functional form of the interaction potential (in the case where only the interaction with nearest neighbor atoms is taken into account, the Poisson ratio is independent of the form of the interatomic interaction and the Young modulus depends only on one characteristic of the interaction, the bond stiffness). All the difficulties indicated above make exact analytical solution of the problem at hand impossible. However, if the interatomic interaction decays fairly rapidly with distance, one can advantageously make use of approximate methods in which the effect of more distant atoms is treated as a perturbation on the situation considered in the previous sections. A detailed discussion of these problems is beyond the scope of this paper. We consider only one particular case, which allows one to appreciate how the inclusion of atoms of the second coordination shell affects the results obtained above.

Let us calculate the Poisson ratio with allowance for the atoms of the second coordination shell by considering the stresses applied along the atomic layers. For the sake of simplicity, we restrict ourselves to the case of a crystal consisting of two atomic layers (Fig. 3; the arrows indicate the atoms with which a given atom interacts). The specific potential energy of the crystal can be written as

$$U = \frac{1}{V_0} \left[ P(a^2) + P\left(\frac{1}{4}a^2 + h^2\right) + P\left(\frac{9}{4}a^2 + h^2\right) \right], \quad (18)$$

where  $P(r^2) \stackrel{\text{def}}{=} \Pi(r)$  is the potential energy of interatomic interaction (as a function of distance squared) and  $V_0$  is the crystal volume per atom. The value of  $V_0$  cannot be defined unambiguously, but this value is not used in what follows. The last term in Eq. (18) [not included in Eq. (17)] describes the interaction with atoms of the second coordination shell. The Poisson ratio for stresses applied along the  $x$  axis can be calculated from Eqs. (8) and (16) to be

$$\nu_1 = -\frac{C_{21}}{C_{22}} = -\frac{\partial^2 U}{\partial \varepsilon_1 \partial \varepsilon_2} \left( \frac{\partial^2 U}{\partial \varepsilon_2 \partial \varepsilon_2} \right)^{-1}. \quad (19)$$

**Table 2.** Calculated Poisson ratio for the case where stresses are applied along the atomic layers

	Allowance for atoms of the first coordination shell alone	Allowance for atoms of the second coordination shell	
		approximate	exact
Poisson ratio	0.333	0.320	0.318
Deviation from $\nu_\infty$ , %	0	4.1	4.5
Computing formulas	(9)	(22)	(20), (21)

Substituting Eq. (18) into Eq. (19) yields

$$\nu_1 = -\frac{a^2 P''\left(\frac{1}{4}a^2 + h^2\right) + 9P''\left(\frac{9}{4}a^2 + h^2\right)}{4h^2 P''\left(\frac{1}{4}a^2 + h^2\right) + P''\left(\frac{9}{4}a^2 + h^2\right)}. \quad (20)$$

The quantities  $a$  and  $h$  should be determined from the equilibrium conditions  $\partial U/\partial a = \partial U/\partial h = 0$ . Using Eq. (18), these conditions can be represented in the form

$$P'(a^2) + 2P'\left(\frac{1}{4}a^2 + h^2\right) = 0, \quad (21)$$

$$P'\left(\frac{1}{4}a^2 + h^2\right) + P'\left(\frac{9}{4}a^2 + h^2\right) = 0.$$

Solving the set of equations (21) and substituting the obtained values of  $a$  and  $h$  into Eq. (20) yields the Poisson ratio. If the interaction potential decays fairly rapidly with distance, we can use an approximate expression,

$$\nu_1 \approx \frac{1}{3} \left( 1 + 8 \frac{P''(3a_0^2)}{P''(a_0^2)} \right), \quad (22)$$

which is obtained from Eq. (20) by replacing  $a$  and  $h$  by their values for the undeformed lattice and expanding the result in powers of the small parameter  $P''(3a_0^2)/P''(a_0^2)$ .

Let us discuss Eq. (22). It will be recalled that in the case of the interaction with nearest neighbor atoms alone, the Poisson ratio  $\nu_1$  was shown to be independent of the number of atomic layers and exactly equal to its macroscopic value,  $1/3$ . It follows from Eq. (22) that the allowance for the interaction with atoms of the second coordination shell leads to a deviation of the value of  $\nu_1$  from  $1/3$ ; however, this deviation is small if the interaction potential decays rapidly with distance. For example, in the case of the Lennard–Jones potential

$$\Pi(r) = P(r^2) = \Pi_* \left[ \left( \frac{a_0}{r} \right)^{12} - 2 \left( \frac{a_0}{r} \right)^6 \right]$$

(where  $a_0$  is the equilibrium spacing in a system of two atoms and  $\Pi_*$  is the binding energy), the value of

$P''(3a_0^2)$  can be as small as 0.5% of  $P''(a_0^2)$ . Substituting this value into Eq. (22), we find that the Poisson ratio changes by 4% when the interaction with atoms of the second coordination shell is included. The numerically calculated values of the Poisson ratio from exact formulas (20) and (21) and from the approximate expression (22) are listed in Table 2.

Thus, allowance for the interaction with atoms of more distant coordination shells leads to changes in the elastic moduli, but these changes are insignificant if the interaction potentials decay rapidly with distance. It should be noted that we made calculations for the case of  $N = 2$ , where the size effect is the most pronounced; for larger values of  $N$ , the influence of the second coordination shell is even less noticeable. However, in a three-dimensional nanocrystal, the effect may be stronger. For example, for an fcc lattice, the distance to the second coordination shell is  $\sqrt{2}a_0$  (instead of  $\sqrt{3}a_0$  as in the two-dimensional case) and the corresponding value of  $P''(2a_0^2)$  for the Lennard–Jones potential is equal to 3% of  $P''(a_0^2)$  (instead of 0.5% in the two-dimensional case).

## 5. DISCUSSION

In the previous sections, we considered the case of a two-dimensional crystal with an hcp lattice infinite in one direction and having a finite number of atomic layers in the other. Now, we will discuss the obtained results and their possible application to crystals of other types.

We established above that there is an ambiguity (of a fundamental nature) in determining the size of a nanocrystal, which leads to uncertainties in many macroscopic characteristics, such as the applied stress, Young modulus, and specific volume strain energy. There is no way to define the nanocrystal size unambiguously; if the size definition is such that the elastic moduli are as close to their macroscopic values as possible, then the Cauchy–Green relations are modified and the elastic constant tensor of the crystal ceases to be symmetric. If, conversely, the Cauchy–Green relations are assumed to be valid, the size effect is enhanced considerably. We note that the ambiguity under discussion does not manifest itself in the values of quantities (such as the Poisson ratio and the strain energy per unit mass) that are independent of the way in which the nanocrystal size is defined.

From the results of our study, it also follows that the anisotropy of the elastic properties depends on the shape and size of the nanocrystal. The mechanical properties of an infinite crystal lattice, as a rule, are anisotropic; however, in the case of a nanocrystal, the anisotropy associated with the structure of the crystal

lattice is combined with the anisotropy related to the shape and size of the nanocrystal.

In the case considered in this paper, the Poisson ratio decreases and the Young modulus increases with decreasing thickness of the nanocrystal. For very thin crystal films, these elastic moduli can differ from their macroscopic values by a factor of two. This conclusion correlates well with the values of the elastic moduli determined from the experimental data from [1], according to which the Young modulus of a thin film increases with decreasing film thickness. However, it should be verified whether or not this conclusion is applicable to crystal lattices of other types (above all, three-dimensional ones).

We also found that if the interaction with atoms of the first coordination shell alone is taken into account, the Poisson ratio is independent of the character of the atomic interaction and the Young modulus depends only on one parameter of this interaction, the bond stiffness. Allowance for the interaction with atoms of the second coordination shell leads to enhancement of the size effect (especially in the three-dimensional case). The elastic moduli become strongly dependent on the functional form of the atomic interaction. These properties are exhibited by both two- and three-dimensional simple crystal lattices. However, if the atomic interaction decays rapidly with distance, the allowance for the interaction with atoms of the second coordination shell leads only to a negligible correction.

Thus, the results of this study allow us to conclude that the continuum mechanics, including the continuum elasticity theory, should be applied to nanocrystals with a great deal of caution. Allowance should be made for the change in the mechanical characteristics when crystals are nanometer sized. This conclusion is especially true for the characteristics (such as the Young modulus) that can be defined differently on a nanometer scale. When such characteristics are used, their definition should be clearly indicated in the case of nanometer-sized objects. However, we do not argue that the classical elasticity theory is completely inapplicable on a nanometer scale. Rather, this theory should be used with allowance for the size effects and the adequacy of the continuum approximation should be verified in each specific case. We note that, according to the calculations presented above, the size effect is more significant when a nanocrystal consists of a few atomic layers; the size effect is small in the case of several tens of atomic layers and is negligible for crystals with hundreds of atomic layers.

The question of how the discreteness of the atomic structure affects the mechanical characteristics is also of importance in the following respect. The molecular dynamics method is presently used widely for modeling macroscopic processes in solids [11–15], and the question arises of how many particles should be taken

into account in calculations in order to obtain the required accuracy. According to our results, the error caused by the replacement of a continuous medium by its discrete atomic analog is roughly  $1/N$ , where  $N$  is the ratio of the characteristic linear dimension of the model to the average interatomic distance. Therefore, for the error to be 1%, we should take 100 particles in one-dimensional modeling,  $10^4$  particles in the two-dimensional case, and  $10^6$  particles in the three-dimensional case. Calculations for such systems can be easily carried out on a modern computer. Therefore, in principle, the molecular dynamics method can be used for modeling the processes in a macroscopic solid.

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