



Fullerite-based nanocomposites with ultrahigh stiffness. Theoretical investigation



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ARTICLE INFO

Article history:

Received 18 November 2016

Received in revised form

30 December 2016

Accepted 10 January 2017

Available online 13 January 2017

ABSTRACT

We present our results of design of a new model of fullerite-based material with ultrahigh mechanical stiffness closely related with experimental data. In this study, we investigated the nature of enhanced mechanical characteristics (i.e. bulk modulus) and establish the relation between geometrical parameters of the model, which allows the estimations of potential conditions for fabrication of superhard material with outstanding mechanical properties. The atomic structure of proposed fullerite-based nanocomposite was analyzed and mechanical properties as a functions of geometrical characteristics were examined in details.

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1. Introduction

Materials harder than diamond always attract attention from the scientific community [1–6]. Therefore, it is not surprising that every experimental confirmation of existence of superhard (hardness is comparable with diamond one) and ultrahard materials (hardness exceeds it) generates a new wave of investigations in the field of research. One of the successful attempts of production the ultrahard material was made by Blank et al. [7,8] with series of the papers, where successful synthesis of ultrahard material called as “tismanit” consisted of 3D-polymerized C₆₀ molecules was reported. Other materials with superior mechanical properties were further synthesized in a number of works, where ultrahard samples based on polymerized fullerene molecules [9,10], graphite [11,12] and amorphous carbon [13] scratch the diamond anvil.

Among the numerous theoretical works [14–22], associating with attempts to clarify the crystal structure of experimentally observed superhard materials, the X-ray diffraction patterns (XRD) of the model proposed by Chernozatonskii et al. [14] (called as SH-phase) agrees very well with experimental data [7]. Nevertheless,

the study of Perottoni et al. [15] concludes that the bulk modulus of SH-phase is significantly lower (about 302 GPa) than experimental value (from 540 to 1700 GPa [7,8]). This distinction might be related with the difference between lattice parameters of the model and fabricated sample, which was under constraint conditions (compressed by more than 6%). It is known from experiments that C₆₀ molecules undergo phase transition in polycrystalline diamond at the pressure higher than 20 GPa [23]. This result allows one to suppose that applied high pressure leads to diamondization of the part of fullerite, while another part remains in the compressed state (SH-phase) with decreased lattice parameters. According to this, we designed the nanocomposite model consisted of grains of SH-phase surrounded by single crystal diamond. We simulated the X-ray diffraction patterns of proposed model depending on the size of fullerite grain and compared it with experimental data. Then we investigated the dependence of mechanical characteristics on the size of fullerite grain and determined the critical grain size wherein the bulk modulus exceeds the diamond value.

2. Computational details

The atomic structure and mechanical properties of newly proposed carbon nanocomposites were studied by the classical molecular dynamics method allowing the consideration of systems consisting of many thousands of atoms. The geometry relaxation

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was carried out using Brenner interatomic potential [24] as implemented in LAMMPS package [25]. To achieve better relaxation the simulation of annealing at temperature decreasing from 500 to 10 K was applied, while the maximum interatomic forces became less or equal to 0.05 eV/Å.

To estimate the bulk modulus from the energy–volume curve, each considered structure was hydrostatically compressed and expanded; at each step, the optimization of geometry was carried out. Then the energy of each structure depending on the unit volume was evaluated and the bulk moduli of all considered structures were found by method of approximation using the Murnaghan equation [26,27]. This approach was tested on single crystal diamond, it was found that calculated data (457 GPa) corresponds well with reference experimental data (445 GPa) [7,8] and theoretical results (445 GPa) [28].

3. Results and discussions

We consider a model of nanocomposite made of the hard grains of SH-phase [14] surrounded by homogeneous diamond environment. SH-phase was chosen as a grain of the nanocomposite because its atomic parameters, XRD pattern and mechanical characteristics are well corresponded to experimental data [7]. The lattice parameters of body-centered orthorhombic fullerite crystal (SH-phase with *Immm* space group) equal to $\mathbf{a} = 0.867$ nm, $\mathbf{b} = 0.881$ nm and $\mathbf{c} = 1.260$ nm while the lattice parameters from experiment are $\mathbf{a} = 0.949$ nm, $\mathbf{b} = 0.780$ nm and $\mathbf{c} = 1.027$ nm [7]. However, it was calculated by Perottoni et al. [15] that lattice parameters of such polymerized fullerite are $\mathbf{a} = 0.866$ nm, $\mathbf{b} = 0.859$ nm and $\mathbf{c} = 1.373$ nm. The difference between calculated lattice parameters allows the assumption that SH-phase considered in Ref. [14] was hydrostatically compressed by ~6% according to experimental data. The bulk modulus of single crystal SH-phase was estimated to be about 800 GPa [14]. Thus, increased bulk modulus of SH-phase might be described by compression, because compression of the material leads to stiffening, represented by an increase in the sound velocities with increasing pressure [20]. Stabilization of shrank fullerite grain by diamond matrix will promote significant augmentation of grain stiffness (higher than stiffness of diamond) and will lead to increasing of mechanical characteristics of whole nanocomposite.

In the designed model of nanocomposite SH-phase is also hydrostatically compressed on the same rate (~6%). Schematic illustration of proposed material and atomic structures of each constituent part are shown in Fig. 1a. We consider single crystal diamond as a hard shell, surrounding the compressed grain of SH-phase, which prevents the removal of compression and relaxation (dilatation) of the grain. A number of different nanocomposites can be considered by choosing different values of the average grain size along \mathbf{a}, \mathbf{b} -axis (S_G) and thickness of diamond shell (h_D) in assumption of periodically arranged grains in the composite. The lattice parameter along c -axis is always about $1.4 \times S_G$ and can be directly calculated. Thus, we used only S_G as a main parameter for description the size of the grains. Also the size can be described by number of polymerized fullerenes in the grain, e.g. smallest possible grain contained only one C_{60} molecule with bridges formed by (2 + 2) and (3 + 3) cycloaddition processes [14] and its size is denoted as $1 \times 1 \times 1$.

Let us study in details the changes of atomic geometry depending on the grain size. Simulated XRD patterns of single crystal SH-phase and proposed nanocomposites with different grain sizes, but with constant thickness of diamond matrix of 2 nm compared to experimental XRD pattern of ultrahard fullerite [7] shown in Fig. 1b. The wavelength of the X-ray source was taken as Cu-K α 1.54 Å according to experimental setup [7].

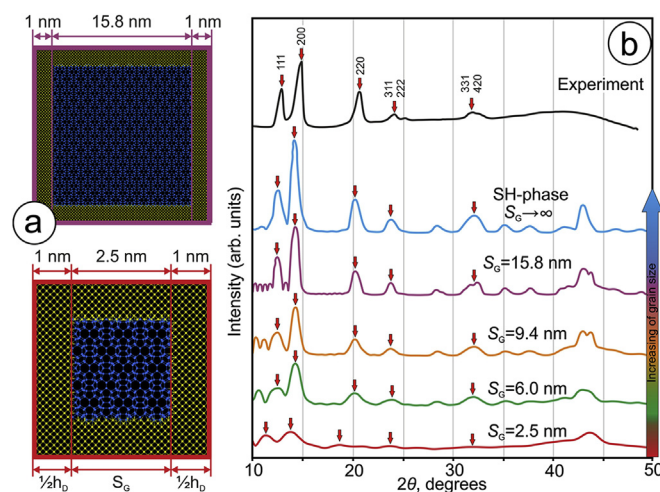


Fig. 1. a) The atomic structure of proposed nanocomposite with smallest ($S_G = 2.5$ nm) and largest ($S_G = 15.8$ nm) considered grain size. Atomic structures of grain consisted of SH-phase is highlighted by blue, surrounded diamond shell is yellow; color of the border corresponds to color of XRD pattern. b) Simulated X-ray diffraction patterns of single crystal SH-phase with reduced atomic parameters fitted to experimental data [7,14] and relaxed nanocomposites with different grain sizes with constant thicknesses of diamond matrix of $h_D = 2$ nm compared to experimental data from Refs. [7,14] (denoted by black). Red arrows indicate the main peaks. (A colour version of this figure can be viewed online.)

The atomic structure of the large nanocomposites models (with size of the grains S_G larger than 15 nm) was not relaxed due to the extremely large number of atoms (more than 10 million). Such huge model cannot be relaxed even using empirical potential approach, but we assume the negligible contribution of interface to the simulated XRD, which structure mainly changes during the optimization. This assumption is supported by ratio between interface and rest atoms equaled to only 0.002.

In Fig. 1b the dependence of XRD patterns on the fullerite grain size is presented. It was found that with increasing of grain size simulated XRD pattern tends to measured spectrum [7] in the region $2\theta < 35^\circ$ (Fig. 1b). The absence of the peak at 44° (associated with (111) reflection of diamond) in the experimental XRD pattern can be explained by the absence of single crystal diamond in the fabricated sample. It can be proposed that experimental sample was surrounded by amorphous sp^3 -hybridized carbon, which indicated by very smooth region from 35° to 45° . With increasing of grain size, the peak at 12° (associated with (111) reflection of SH-phase) becomes more distinguishable and the relative intensities of peaks located at 12° and 14° (associated with (200) reflection of SH-phase) become closer to experimental. It should be noted that intensity of peak at 21° appears from the grain size about 6 nm and increases with the grain size increasing from 6 nm followed by the approach to the corresponding experimental data at grain size of 15.8 nm. Small peaks at 24° and 32° associated with (311), (222) and (331), (420) reflections, respectively appear after the grain size reaches the value of 6 nm. Thus, X-ray diffraction pattern from grain size 6 nm begins to display the characteristics features of the experimental spectra, whereas from 15.8 nm grain size it becomes practically equal to XRD pattern of simulated single crystal SH-phase as well as experimental data [7].

Then we proceeded to the detailed investigation of mechanical properties of proposed nanocomposites. From $S_G \geq 6$ nm our data displays visible correspondence with experiment. We studied nanocomposites with the grains varies from $1 \times 1 \times 1$ ($S_G = 0.9$ nm) to $8 \times 8 \times 8$ ($S_G = 7.1$ nm) polymerized C_{60} molecules (see Fig. 1a). Surrounded diamond matrix had constant thickness of $h_D = 2$ nm and grains were hydrostatically compressed on ~6%.

The bulk modulus describes the ability of an object to change its volume under the influence of uniform hydrostatic compression. Applying the hydrostatic compression and dilatation of single crystal SH-phase in a wide range from -24% to 8% allows the calculation of the dependence of bulk modulus on the uniform strain, shown in Fig. 2a, where the points are calculated values of bulk modulus. Uncompressed SH-phase reveals bulk modulus of 236 ± 21 GPa. Compression leads to stiffening of the material with increasing of its bulk modulus. It was estimated that value of bulk modulus of single crystal SH-phase compressed by 6% equal to 624 ± 23 GPa (0.6 TPa in Fig. 2a), which agrees well with earlier estimations [14].

The behavior of bulk modulus (B_0) of considered nanocomposites with constant thickness of diamond matrix ($h_D = 2$ nm) depending on the size of fullerite grains was studied in details. Due to variability in atomic geometries of nanocomposites, we performed 10 computational tests for each of the sizes and plotted the obtained data in Fig. 2b. As one can see, carbon nanocomposite with the smallest grain size of $S_G = 0.9$ nm ($1 \times 1 \times 1$ supercell) displays bulk modulus $B_0 = 430 \pm 50$ GPa, which does not exceed the calculated bulk modulus of single crystal diamond 457 GPa. Further increasing of grain size from $S_G = 1.7\text{--}3.5$ nm ($2 \times 2 \times 2$ to $4 \times 4 \times 4$ supercells, respectively) leads to significant increasing of bulk modulus up to 870 ± 99 GPa at $S_G = 3.5$ nm (Fig. 2b). Nanocomposites with larger grain sizes (>3.5 nm) reveal bulk modulus of 1027 ± 111 GPa ($S_G = 4.4$ nm). Further increasing leads to slight fluctuations of bulk modulus around 1100 GPa. Obtained data with compressed fullerite grains displays a great augmentation of bulk modulus compared to single crystal diamond, which closely relates to experimental data [7,8]. Thus, we found that with increasing of grain size, the bulk modulus of the nanocomposite increases as well up to 1096 ± 157 GPa and then after the plateau ($S_G = 4.4\text{--}6.2$ nm) bulk modulus monotonically decreases. The dominant impact to mechanical characteristics of whole nanocomposite will come mainly from fullerite rather than from diamond and, therefore, bulk modulus will tend to the bulk modulus of single crystal SH-phase with increasing of the size of fullerite grains in the nanocomposite.

It should also be noted that mechanical characteristics of composites significantly depend on the relation between thickness of diamond matrix and size of fullerite grain. Let us pay attention on this effect in more details. The lattice parameters of SH-phase as a grain of different sizes inside the nanocomposite with constant thickness of diamond matrix $h_D = 2$ nm is shown in Fig. 2c, where each size of the grain corresponds to a certain color of the bars. The lattice parameters *a*, *b* and *c* denote by the letters on the sets of bars. The lattice parameters of single crystal SH-phase (*a* = 0.867 nm, *b* = 0.881 nm and *c* = 1.260 nm) are marked by white horizontal lines. For grain sizes from $1 \times 1 \times 1$ ($S_G = 0.9$ nm) to $2 \times 2 \times 2$ ($S_G = 1.7$ nm) supercells, lattice parameters *a* and *c* are less than those for single crystal SH-phase. It can be explained by relatively large thickness of diamond shell (2 nm) with respect to the grains ($S_G = 0.9$ and 1.7 nm, respectively). The higher value of lattice parameter *b* in composite with single fullerite grain can be explained by the mismatch between diamond lattice parameter and fullerite ones. Increasing the size of fullerite grain from 2.6 nm ($3 \times 3 \times 3$ supercell) leads to decreasing of the lattice parameter *b* caused by decreasing of lattice mismatch. However, only for grain size of $3 \times 3 \times 3$ ($S_G = 2.6$ nm) supercell, lattice parameters become equal to single crystal SH-phase compressed by 6% . Further increasing of grain sizes (thickness of diamond matrix is constant and equals 2 nm) leads to increasing of lattice parameters of fullerite, which corresponds to the expansion of grain and reduction of compression ratio inside the diamond matrix. Relatively big size of fullerite grain allows it to release compression inhomogeneously: greater relative expansion observed along *a,b*-axis rather than

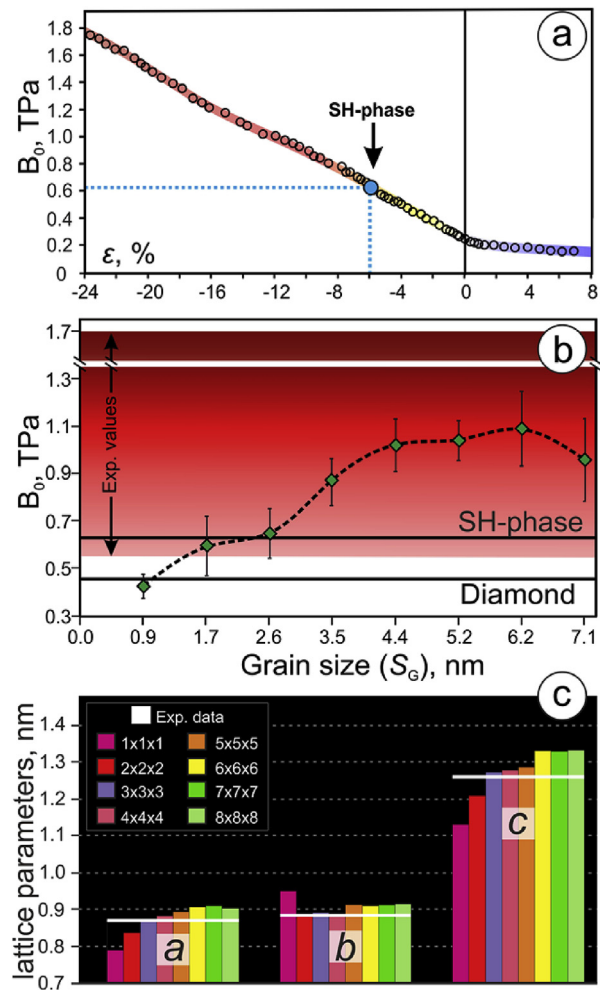


Fig. 2. a) The dependence of bulk modulus of single crystal SH-phase on the uniform strain. The line is guided to the eye; b) Bulk modulus of proposed nanocomposites as a function of grain size compressed by 6% with the thickness of diamond matrix $h_D = 2$ nm. The range of experimental values of the bulk modulus ($540\text{--}1700$ GPa) taken from Refs. [7,8] is indicated by red gradient. The calculated bulk modulus of single crystal SH-phase compressed by 6% and single crystal diamond are marked by black horizontal lines; c) Lattice parameters *a*, *b*, *c* of SH-phase inside the diamond matrix (grain of nanocomposite) for different sizes of the grain (each size corresponds to bar with a certain color). White horizontal lines are experimental values [7]. (A colour version of this figure can be viewed online.)

along *c*-axis (see Fig. 2c). Thus, considering nanocomposites with big sizes of the grains ($S_G > 2.6$ nm) and $h_D = 2$ nm, one will not obtain great augmentation of bulk modulus due to release of the stress inside the grains caused by relatively big S_G compared to h_D .

Taking into account the previous conclusion, the particular high value of bulk modulus of nanocomposite could be obtained using the relation between size of fullerite grain (S_G) and thickness of diamond matrix (h_D). Varying of fullerite and diamond sizes with respect to each other may significantly influence to mechanical characteristics. Thus, we proposed the simple relation between sizes of diamond and fullerite, as a ratio h_D/S_G , to constantly obtain nanocomposites with superior mechanical characteristics compared to the value of single crystal SH-phase within the experimental range of $540\text{--}1700$ GPa [7,8]. We considered a number of nanocomposites with closest to experiment bulk moduli and calculate h_D/S_G ratio. Estimations of h_D/S_G ratio of such structures with closest to experiment bulk moduli gave us a ratio equals 0.77 . This fact means, that any structures with $h_D/S_G = 0.77$ would reveal bulk modulus equal to bulk modulus of single crystal SH-phase (624 ± 23 GPa) within the

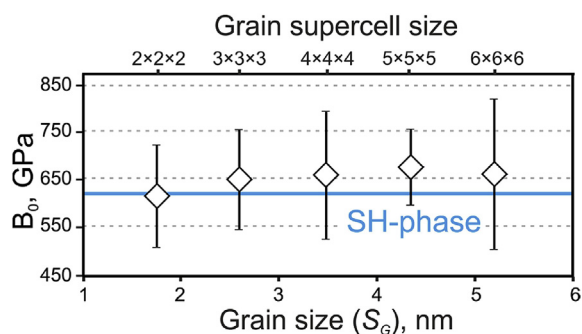


Fig. 3. The dependence of bulk modulus on the grain size of nanocomposites with $h_D/S_G = 0.77$. Calculated value of bulk modulus of single crystal SH-phase is marked by horizontal line. (A colour version of this figure can be viewed online.)

experimental range of 540–1700 GPa [7,8]. We consider five nanocomposites with grain sizes of 1.7, 2.6, 3.5, 4.4 and 5.2 nm with the thickness of diamond matrix that satisfies the relation $h_D/S_G = 0.77 \pm 0.05$. Calculated bulk moduli of considered structures are shown in Fig. 3. It should be noted that all calculated nanocomposites with $h_D/S_G = 0.77 \pm 0.05$ display similar values of bulk modulus hovering around the value of SH-phase (Fig. 3). Thus, we can propose that grains of SH-phase with experimentally measured lattice parameters independently on size (more than $1 \times 1 \times 1$) can yield the bulk modulus close to SH-phase value and much higher than for the bulk diamond.

4. Conclusions

In this work we proposed new model of carbon nanocomposite based on polymerized body-centered orthorhombic fullerite (grain) and single crystal diamond (shell) displaying ultrahigh stiffness. Atomic structure was examined in details in terms of simulated XRD patterns for composites with different sizes and compared with reference experimental data. It was found that XRD pattern becomes as closer to experimental data as the grain size becomes larger and begins to display the characteristics features of the experimental spectra from the grain size larger than 6 nm. Bulk moduli of nanocomposites with different grain sizes were calculated showing enhanced values compared to single crystal diamond (up to 1 TPa) caused by the compression of fullerite inside the diamond matrix. Mechanical stiffness of the nanocomposites with lattice parameters close to experimentally measured values was examined. We found that grains even with smaller size than 6 nm (but larger than single fullerene molecule) can yield the nearly constant bulk modulus close to value of bulk SH-phase and much higher than for the bulk diamond. We hope that the present study can be considered as another step toward the controllable fabrication of carbon nanocomposites with constant superior mechanical stiffness exceeding diamond value.

Acknowledgments

The work was supported by the Grant of President of Russian Federation for government support of young PhD scientists (MK-6218.2015.2). Authors sincerely appreciate Dr. D.G. Kvashnin for the fruitful discussion of the work results. P.B.S. gratefully acknowledges the financial support of the Ministry of Education and Science of the Russian Federation in the framework of Increase Competitiveness Program of NUST «MISI» (N^o K2-2015-033) and Government Task, project #3556. L.A.C. acknowledges EU Marie Curie International Research Staff Exchange Scheme Fellowship within the 7th European Community Framework Programme (MC-IRSES

proposal 318617 FAEMCAR project).

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