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Potential superhard osmium dinitride with fluorite and pyrite structure: First-principles calculations

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We have performed systematic first-principles calculations on dicarbide, -nitride, -oxide, and -boride of platinum and osmium with the fluorite structure. It is found that only PtN_2, OsN_2, and OsO_2 are mechanically stable. In particular, OsN_2 has the highest bulk modulus of 360.7 GPa. Both the band structure and density of states show that the new phase of OsN_2 is metallic. The high bulk modulus is owing to the strong covalent bonding between Os 5d and N 2p states and the dense packed fluorite structure. In addition, the total-energy calculation for pyrite structure has also been performed, which indicates its mechanical and energetic stability but much lower bulk modulus compared to the fluorite structure.

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The search for hard materials compared to or even harder than diamond, which has the highest measured hardness of 96 GPa (Ref. 1) and bulk modulus of 443 GPa,[2] has a long history and has stimulated a variety of great achievements in high-pressure research.[3–6] Consequently, many new superhard materials have been prepared by high-pressure techniques, especially after the laser-heated diamond-anvil cells was invented. In general, two groups of materials are powerful candidates for superhard materials: (i) strong covalent compounds formed by light elements, such as polymorphy of C_3N_4,[7] B_6O,[8] and c-BC_2N.[9] (ii) Partially covalent heavy transition metal boride, carbide, nitride, and oxide. RuO_2 (Ref. 10) and OsB_2 (Ref. 11) are such examples. Theoretically, the nature of hardness has been extensively investigated and many new models have been proposed.[1,3,12–16] For the strong covalent materials, hardness can be directly derived,[13–16] while for some metallic transition metal-based superhard materials, it is acknowledged that bulk modulus or shear modulus can measure the hardness in an indirect way.[1,12,17] That is, materials with high bulk or shear modulus are likely to be hard materials.

In the present paper, we focused on the bulk modulus, mechanical, and energetic stability of osmium dinitride (OsN_2) with fluorite structure[18] by calculating the elastic constants within the density functional based electronic structure method.[19] We report that the proposed OsN_2 compound has very high value of bulk modulus (360.7 GPa) which is even higher than that of OsO_2 with the same structure (347.5 GPa) and is comparable with that of orthorhombic OsB_2 [365–395 GPa (Ref. 11)].

All first-principles calculations were performed with the CASTEP code.[20] The ultrasoft pseudopotential[21] was employed to describe the interaction between ions and electrons. Both the local-density approximation (LDA) (Ref. 22) and the generalized gradient approximation (GGA) (Ref. 23) were used to describe the exchange and correlation potentials. For the Brillouin-zone sampling, the Monkhorst-Pack (MP) scheme with a grid of 0.03 Å^{-1} was adopted.[24] The plane-wave cutoff energy is chosen to be 550 eV for LDA and 500 eV for GGA calculations. For the self-consistent field iterations, the convergence was assumed when (i) the total energy difference between the last two cycles was less than 1×10^{-6} eV/atom; (ii) the maximal force on each atom was below 0.006 eV Å^{-1}; and (iii) the maximal atomic displacement was below 2×10^{-4} Å. We have tested that with even more strict parameters the total energy can be converged within 0.002 eV/atom for all the systems studied. After getting the equilibrium geometry configuration, we applied the so-called "stress-strain" method to obtain the elastic constants in that the stress can be easily obtained within the density functional based electronic structure method.[25] The stress-strain relation can be described as

$$(\sigma_1,\sigma_2,\sigma_3,\sigma_4,\sigma_5,\sigma_6) = C(\varepsilon_1,\varepsilon_2,\varepsilon_3,\varepsilon_4,\varepsilon_5,\varepsilon_6)^T. \quad (1)$$

For the cubic crystal, there are only three nonzero independent symmetry elements (c_{11}, c_{12}, and c_{44}). Applying two kinds of cubic distortions (ε_1 and ε_4) along the crystallographic directions shown in Figs. 1(a) and 1(b), respectively, can give stresses relating to these three elastic coefficients, yielding an efficient method for obtaining elastic constants for the cubic system. For the hexagonal crystal, there are five independent symmetry elements (c_{11}, c_{12}, c_{13}, c_{33}, and c_{44}). In order to obtain the additional components c_{13} and c_{33}, another monoclinic distortion [ε_3, see Fig. 1(c)] is needed. For each strain, in our practical calculations, its value is var-

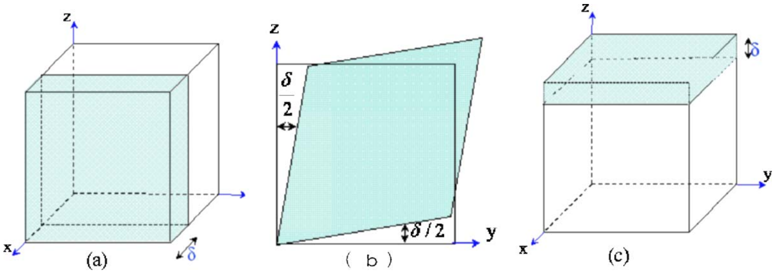

FIG. 1. (Color online) The schematic of strain types: (a) ε_1; (b) ε_4; (c) ε_3.

ied from −0.003 to +0.003 with a step of 0.0012, then each of three elastic constants takes the arithmetic average value of the six steps. The bulk modulus is obtained from the elastic constants by the relation $B=(c_{11}+2c_{12})/3$.

The lattice and elastic constants of diamond, pure platinum, hexagonal, and cubic pure osmium were calculated to verify the reliability of the present calculations. It is well known that LDA usually underestimates the lattice constants and overestimates the elastic constants, while GGA overestimates the lattice constants and underestimates the elastic constants.[26,27] For this reason we adopted to use the average of the LDA and GGA results as our theoretical estimates. As shown in Table I, the theoretical average lattice constant and bulk modulus of diamond are 3.546 Å and 446.5 GPa, which agree well with the experimental values of 3.567 Å (Ref. 12) and 443 GPa,[2] with an error of 0.59% and 0.79%, respectively. For the cubic osmium and cubic platinum, the theoretical bulk modulus values (Pt: 287.2 GPa, Os: 418.8 GPa) are also in accordance with other theoretical results [Pt: 279 GPa,[26] Os: 417.1 GPa (Ref. 28)]. With regard to the hexagonal Os, as shown in Table I, the calculated equilibrium lattice parameter c/a is 1.581, in good agreement with the experimental value of 1.580.[29,30] The calculated bulk modulus for hexagonal Os is 424.0 GPa, which is also in accordance with previous theoretical results [403 GPa,[31] 429.2 GPa (Ref. 28)] and experimental measurements [462±12 GPa,[29] 411±6 GPa,[32] 395±15 GPa (Ref. 33)]. Based on above-mentioned accordance, therefore, we believe that the plane-wave ultrasoft pseudopotential (PW-PP) method we employed is reliable in investigating the mechanical properties of osmium and platinum compounds.

Now we turn to fully study OsN_2 with fluorite structure. The results of lattice constant, elastic constants, and bulk modulus of OsN_2 are listed in Table II. For comparison, we have in addition given a calculation on platinum dinitride (PtN_2) and osmium dioxide (OsO_2), and the results are also listed in Table II. Given the elastic constants and bulk modulus, the shear modulus G and the Young's modulus E can be deduced as follows: $G=(c_{11}-c_{12}+2c_{44})/4$, $E=9BG/(3B$

TABLE I. The calculated equilibrium lattice parameters a (Å), elastic constants c_{ij} (GPa), bulk modulus B (GPa), polycrystalline shear modulus G (GPa), Young's modulus E (GPa), and Poisson's ratio ν of typical pure crystals. The boldface numbers represent the theoretical estimations of bulk modulus by present calculations.

		a	c_{11}	c_{33}	c_{44}	c_{13}	c_{12}	B	G	E	ν
Diamond	LDA	3.525	1105.8		607.3		140.5	462.3	545.0	1173.8	0.08
	GGA	3.566	1053.3		569.1		119.5	430.7	518.0	1109.3	0.07
	Ave.	3.546	1079.6		588.2		130.0	**446.5**	531.5	1141.6	0.08
	Expt.	3.567[a]						443[b]			
Pt (fcc)	LDA	3.921(3.890[c])	391.1		82.3		279.0	316.4(320[c])	69.2	193.5	0.40
	GGA	3.998(3.967[c])	307.9		65.7		232.9	257.9(238[c])	51.6	145.1	0.41
	Ave.	3.960(3.928[c])	349.5		74.0		256.0	**287.2**(279[c])	60.4	169.3	0.41
	Expt.	3.924[d]						276[e]			
Os (fcc)	LDA	3.798(3.814[f])	686.9		361.3		323.1	444.4(441.3[f])	271.6	676.9	0.25
	GGA	3.851(3.851[f])	614.7		328.0		282.5	393.2(392.9[f])	247.1	612.9	0.24
	Ave.	3.824(3.841[f])	650.8		344.7		302.8	**418.8**(417.1[f])	259.4	644.9	0.25
Os (hcp)	LDA	2.712	808.7	888.6	271.2	264.7	243.7	449.0			
	GGA	2.750(2.746[a])	730.1	798.3	246.9	230.5	209.8	398.9			
	Ave.	2.731	1538.8	843.5	259.1	247.6	226.8	**424.0**			
	Expt.	2.7313[g]						395,[g] 462[h]			

[a] Reference 12.

[b] Reference 2.

[c] References 26 and 37.

[d] Reference 47.

[e] Reference 48.

[f] Reference 28.

[g] Reference 33.

[h] Reference 29.

TABLE II. The calculated equilibrium lattice parameters a (Å), elastic constants c_{ij} (GPa), bulk modulus B (GPa), polycrystalline shear modulus G (GPa), Young's modulus E (GPa), and Poisson's ratio ν of some fluorite and pyrite crystals. The boldface numbers represent the theoretical estimations of bulk modulus by present calculations.

		a	c_{11}	c_{44}	c_{12}	B	G	E	ν
OsO_2 (fluorite)	LDA	4.770(4.763[a])	721.3	243.1	206.6	378.2(411,[a] 392[b])	250.2	615.0	0.23
	GGA	4.861	632.2	211.2	158.9	316.7	223.9	543.6	0.21
	Ave.	4.816	676.8	227.0	182.8	**347.5**	237.1	579.3	0.22
PtN_2 (fluorite)	LDA	4.943(4.866[c])	499.9	87.4	232.6	321.7(316[c])	110.5	297.4	0.35
	GGA	5.040(4.958[c])	427.9	77.5	188.6	268.3(264[c])	98.6	263.5	0.34
	Ave.	4.992(4.912[c])	463.9	82.5	210.6	**295.0**(290[c])	104.6	280.5	0.35
PtN_2 (pyrite)	GGA	4.874(4.875[d])	689	129	102	297.8(278[d])	211.3	512.7	0.21
	GGA[e]	4.862	668	99	167	272	184	452	0.23
OsN_2 (fluorite)	LDA	4.781	544.5	103.9	309.8	388.0	117.4	319.9	0.36
	GGA	4.856	465.4	79.7	267.3	333.3	89.4	246.2	0.38
	Ave.	4.819	505.0	91.8	288.6	**360.7**	103.4	283.1	0.37
OsN_2 (pyrite)	GGA	4.925	523	107	213	316	131	345.3	0.32

[a]Reference 35.
[b]Reference 36.
[c]References 26 and 37.
[d]Reference 42.
[e]Reference 41.

$+G$), and $\upsilon = E/(2G) - 1$. These quantities are also shown in Table II.

The key criteria for mechanical stability of a crystal is that the strain energy must be positive,[34] which means in a hexagonal crystal that the elastic constants should satisfy the following inequalities:

$$c_{44} > 0, c_{11} > |c_{12}|, \quad (c_{11} + c_{12})c_{33} > 2c_{13}^2, \qquad (2)$$

while for a cubic crystal,

$$c_{44} > 0, c_{11} > |c_{12}|, \quad c_{11} + 2c_{12} > 0. \qquad (3)$$

It is straightforward to verify from Table I that the elastic constants of the hexagonal osmium satisfy formula (2), implying the stability of hcp Os, which is consistent with the experimental observation. In the same manner, from our calculation results in Table II, one can find that PtN_2, OsN_2 and OsO_2 with fluorite structure are also mechanically stable since their elastic constants fit well in formula (3). The stability of these three crystals can also be confirmed by providing the Poisson's ratio, whose value is usually between -1 and 0.5, corresponding to the lower and upper limit where the materials do not change their shapes. Note that the present result of bulk modulus of PtN_2 is 295.2 GPa. The previous full-potential linearized augmented plane waves calculation gives 290 GPa.[26] Remarkably, the two approaches agree well, suggesting again the reliability of PW-PP method in exploring the structural properties of transition metal compounds. On the other hand, we obtained the bulk modulus of OsO_2 to be 347.5 GPa, which is ~13% smaller than that obtained from the full-potential linear muffin-tin orbital method.[35,36] This difference may come from different density functional based electronic structure method. It reveals in Table II that OsN_2 has the highest bulk modulus of 360.7 GPa in our series of calculations; this value of OsN_2 is much higher than that of other noble metal dinitride (347 GPa for IrN_2, 190 GPa for AgN_2, and 222 GPa for AuN_2 (Ref. 37). The shear modulus of OsN_2 is calculated to be 103.4 GPa, comparable with that of PtN_2 (104.6 GPa) as shown in Table II, but much smaller than those of diamond (531.5 GPa) and OsO_2 (237.1 GPa). Thus compared to diamond or OsO_2, OsN_2 cannot withstand the shear stress to a large extent. It is interesting to point out that OsN_2 was implicitly referred to in Ref. 37 to be unstable or a little bulk modulus.[38]

Furthermore, the electronic structure and chemical bonding of OsN_2 with fluorite structure are studied by calculating its total charge density, Mulliken population, and density of state (DOS). In Fig. 2, we plot the total electron density in a $(\bar{1}10)$ plane which cut through both the Os and N sites. The bonding behavior of OsN_2 can be effectively revealed by analyzing the charge density data in real space $\rho(r)$ at three types of crystalline symmetry points, as indicated by filled circles, open squares, and open circles in Fig. 2. We found that the charge density of these three kinds of points are about 0.8, 0.3, and $0e$ Å^{-3}, respectively. Thus the charge density maximum lies between Os and N atoms, indicating formation of strong covalent bonding between them. Combining the fact that each N atom occupies the tetrahedral interstitial formed by four Os atoms around it, it is not difficult to understand that OsN_2 has a low compressibility. Table III shows bond Mulliken population analysis of OsN_2, OsO_2, and PtN_2. It indicates that for these three kinds of materials the bonding is formed between metal atom and nonmetal

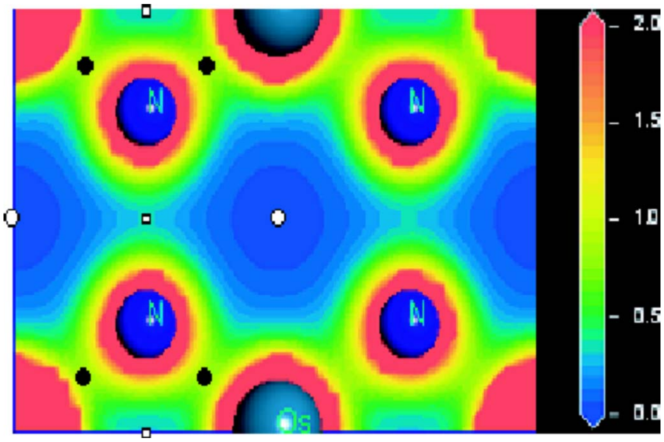

FIG. 2. (Color online) Total electron density of OsN_2 at the $(\bar{1}10)$ plane. The density at three types symmetry points (they are labeled with filled circles, open squares, and open circles) are approximately 0.8, 0.3, and $0e$ Å^{-3}.

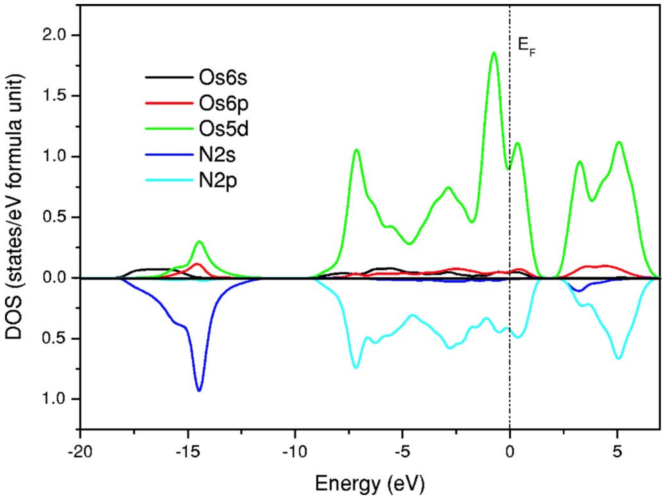

FIG. 3. (Color online) Partial densities of states of OsN_2.

atom, while a weak bonding is formed between two nonmetal atoms. This is compatible to the analysis of the electron density of OsN_2 in Fig. 2. Table III also lists the Mulliken atomic population analysis results, from which we can see the total charge transfer from Os to N is 1.10, resulting Os in +1.10 charge state and N −0.55 charge state. Therefore, the chemical bonding between Os and N has some character of ionicity. Table III shows that the transferred charge in $\mathrm{O}s\mathrm{N}_2$ is almost the same as that in OsO_2, and is more than that in PtN_2. Thus we can make a conclusion that the charge transfer effect is more influenced by the metal atom rather than the nonmetal atom. It is interesting to note that the mechanical properties of OsN_2 are also very similar to OsO_2 rather than PtN_2, as revealed in our above discussions.

The partial DOS is shown in Fig. 3; no energy gap near the Fermi level is seen, indicating the metallic nature of OsN_2. At the Fermi level the total DOS is 1.88 states/ev formula units. It reveals that from −18 to −12 eV the states are mainly N (2s) states with a small contribution from Os (5d and 6p). The states above −9 eV mainly come from Os 5d and N 2p orbitals.

It was recently demonstrated in both theory and experiment that the synthesized platinum nitride crystallized in pyrite structure.[39–42] The pyrite structure (space group number 205), which was also observed in the silica recently,[43] is cubic with 12 atoms per primitive cell. For pyrite PtN_2, both the four Pt atoms and the midpoints of the four nitrogen pairs arrange in fcc positions and result in a NaCl-type arrangement. In addition, each pair of nitrogen atoms aligns along one of the (111) directions. Besides the lattice constant a, the position (u,u,u) of N is the only free structural parameter of pyrite PtN_2. Inspired by these advances, we have also performed a series of *ab initio* total-energy calculations to find if OsN_2 favors the intriguing pyrite structure as platinum nitride does. Figure 4(a) gives the energy of OsN_2 with the internal parameter u varied from 0.23 to 0.40. The plot reveals that fluorite OsN_2 lies at a local minimum, indicating its metastable nature. The location of lowest total energy is at 0.3614 for GGA calculations, corresponding to the lattice constant of 4.9246 Å of the pyrite structure. The bond length of nitrogen pairs in pyrite OsN_2 is found to be 1.365 Å, even smaller than that of pyrite PtN_2 (1.51 Å). The separation of nitrogen pairs in the pyrite OsN_2 and PtN_2 is nearly the same as that of a single-bonded cubic-gauche structure of N observed recently,[44,45] which means that the nitrogen pairs probably consist of some characteristics of covalent bonding. The calculated formation energies of pyrite and fluorite OsN_2 at an ambient pressure are 0.69 and 1.10 eV (per formula unit), which are smaller than those of pyrite PtN_2 (0.72 eV) and fluorite PtN_2 (3.5 eV), respectively. Figure 4(b) plots the enthalpy vs pressure for the fluorite and pyrite structures of

TABLE III. The calculated atomic and bond Mulliken population analysis of OsN_2, OsO_2, and PtN_2. NM1 and NM2 denote the first and second nonmetal atoms, and M denotes the metal atom.

	Atomic (e)			Bond (e)		
	NM1	NM2	M	NM1-M	NM2-M	NM1-NM2
OsN_2	−0.54	−0.54	1.09	1.25	1.25	−0.7
OsO_2	−0.55	−0.55	1.10	0.98	0.98	−0.45
PtN_2	−0.45	−0.45	0.9	1.08	1.08	−0.34

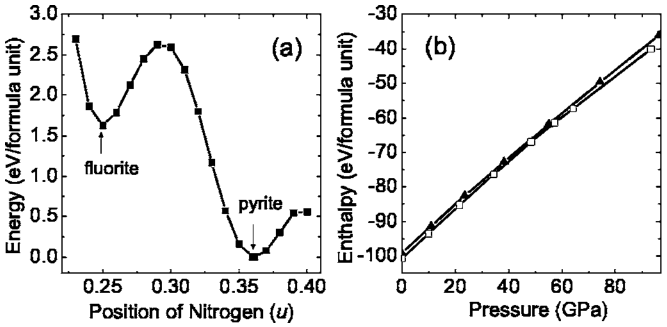

FIG. 4. (a) Total energy of OsN_2 versus the internal parameter u; (b) Enthalpy vs pressure for the fluorite and pyrite structures of OsN_2.

OsN_2. In the overall range of external pressure that we have studied, the enthalpy of pyrite OsN_2 is always lower than that of fluorite OsN_2, implying that no first-order phase transition might occur at zero temperature between these two structures. In addition, the elastic constants of pyrite OsN_2 and PtN_2 are also calculated and listed in Table II, wherein the results for PtN_2 show good agreement with those of experimental and other available theoretical results. The calculated elastic constants of pyrite OsN_2 satisfy formula (3). Therefore, it is also a mechanically stable crystal structure though its bulk modulus is about 10% lower than that of fluorite OsN_2.

In conclusion, the OsN_2 with fluorite structure is first reported to be mechanically stable and have a very high bulk modulus of 360.7 GPa by the first-principles calculations. The electronic and chemical bonding properties have been investigated, indicating that the bonding is a mixture of covalent and ionic components. It is found that the electronic properties of OsN_2 are very similar to that of PtN_2 with the same structure. As a pyrite-type PtN_2 and a orthorhombic-type OsN_2 have been very recently synthesized under high pressure and high temperature conditions,[41,46] we expect that the OsN_2 as well as PtN_2 with fluorite structure may be experimentally prepared in the future.

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