Temperature Dependent Elastic and Ultrasonic Properties of Superhard Metal and its Carbide and Nitride: Os, OsC, and OsN

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Abstract : ***In present investigation, we studied elastic and ultrasonic properties of Os, OsC and OsN in the temperature range 0K to 300K. The second and third order elastic constants have been computed using Coulomb and Born-Mayer potential upto second nearest neighbourhood. The evaluated values of SOEC and TOEC have been applied for finding ultrasonic velocity and ultrasonic Grüneisen parameter. For testing mechanical behaviour, we also computed bulk modulus (B), shear modulus (G), Young modulus (Y), Poisson ratio (ν), anisotropic ratio (A) and tetragonal moduli (C_S) were also computed. Since G/B<0.591 for all materials, hence they have ductile nature. The obtained results are analysed with different types of materials***

Keywords: Elastic constants, ultrasonic velocity, Grüneisen parameters

1. Introduction

Although there are several methods to evaluate the second and third order elastic constants (SOECs & TOECs). The first principle methods are also available for computing the higher order elastic constants, but we have to use a simple method, which gives a clear physical picture *i.e.*, Coulomb and Born Mayer potential. Designing and searching for ultraincompressible and superhard materials is always of great interest due to its variety of industrial applications [1]. The superhard materials [2] like Os, OsC, OsN have a great importance for engineering applications in various fields especially for mechanical applications. Some results of these materials are available in literature.

Elastic and ultrasonic studies have been done theoretically and experimentally in all types of crystals like dielectrics [3] , semiconductors [4], metals [5], semimetallics [6], superconductors [7] and nanomaterials [8]. In solids there are several studies along different crystallographic directions like <100>,<110>, <111> at various temperatures. In present work mechanical and thermal properties of Os, OsC, OsN have been studied in the temperature range 100K-500K.

2. Theory

We used Coulomb and Born -Mayer potential [9] for finding SOECs and TOECs of Os, OsC, OsN.

$$\phi(R) = \phi(C) + \phi(B)$$

Where $\phi(C)$ is the Coulomb potential and $\phi(B)$ is the Born-Mayer potential, given by $\phi(C) = \pm \frac{e^2}{r}$ and

$$\phi(B) = \exp(-\frac{r}{b})$$

Where e is the electronic charge, r is the nearest neighbour distance, b is the hardness parameter and A is the strength parameter.

Following Brugger's definition of elastic constants at absolute zero the SOECs and TOECs are obtained. We get SOECs and TOECs at particular temperature [10] by adding vibrational energy contribution to the static elastic constants *i.e.*,

$$C_{ij} = C^0_{ij} + C_{ij}^{vib}$$

$$C_{ijk} = C^o_{ijk} + C^{vib}_{ijk}$$

Here 0 and vib represents the static and vibrational contribution of elastic constants. The detail expression for for C_{ijk} and C_{ij} are given in our previous paper [11]. Expressions for various mechanical constants like bulk modulus (B), shear modulus(G), Young modulus(Y), Poisson ratio(ν), anisotropic ratio(A), toughness to fractor ratio (G/B) and tetragonal moduli (C_S) are given in our previous paper [6].

The ultrasonic velocities along the <100>, <110>, <111> orientations are of three types i.e. V_L, V_{S1}, V_{S2}; here L and S stands for longitudinal and shear mode of propagation. The expressions for finding the values of ultrasonic velocities are given in literature [12].

Ultrasonic Grüneisen parameters (UGP) play a vital role in the study of thermo elastic properties of the materials. A number of anharmonic properties of solids are frequently expressed in terms of UGP. Brugger [13, 14] derived the expression for the components of Grüneisen tensor in terms of an isotropic elastic continuum. The UGPs and higher elastic constants are related to each other along different directions as given in literature [15].

3. Results and Discussion

The SOECs and TOECs are calculated in the temperature range 0-500K using the Coulomb and Born- Mayer potential with two basic parameters, the nearest neighbour distance and the hardness parameter and are presented in Table 1.

Table 1: Second and third order elastic constants of Os, OsC, OsN at the temperature range 0 to 500K [in the unit of 10^{10} N/m^2]

Material	Temp	C_{11}	C_{12}	C_{44}	C_{111}	C_{112}	C_{123}	C_{144}	C_{166}	C_{456}	C_{44}/C_{12}
Os	0K	7.6559	7.9553	7.9553	-104.10	-31.938	11.456	11.456	-31.938	11.456	1.000
	100K	7.9798	7.8795	7.9873	-105.60	-31.749	11.184	11.506	-32.057	11.456	1.0137
	200K	8.2811	7.8446	8.0142	-107.24	-31.634	11.080	11.535	32.170	11.456	1.0216
	300K	8.5961	7.8097	8.0422	108.97	31.523	10.971	11.565	-32.291	11.456	1.0290
	400K	8.9146	7.7747	8.0704	-110.73	-31.412	10.862	11.594	-32.411	11.456	1.0380
	500K	9.2344	7.7397	8.0988	-112.49	-31.301	10.752	11.624	-32.532	11.456	1.0464
OsC	0K	7.2595	4.7411	4.7411	-104.20	-19.317	7.1099	7.1099	-19.317	.1099	1.0000
	100K	7.7024	4.6163	4.7738	-106.51	-19.043	6.4969	7.1719	-19.447	7.1099	1.0341
	200K	7.8777	4.5710	4.7738	-107.36	-18.838	6.3790	7.1948	-19.499	7.1099	1.0471
	300K	8.1254	4.5934	4.8028	-108.85	-18.683	-6.263	7.2159	-19.574	7.1099	1.0718
	400K	8.3941	4.4974	4.8204	-110.52	-18.539	6.1407	7.2371	-19.656	7.1099	1.0718
	500K	8.6714	4.4610	4.8384	-112.25	-18.397	6.0152	7.2586	-19.740	7.1099	1.0846
OsN	0K	6.6574	4.7779	4.7779	-94.356	-19.415	7.0967	7.0967	-19.415	7.0967	1.0000
	100K	7.0469	4.6671	4.8090	-96.303	-19.172	6.5786	7.1551	-19.536	7.0967	1.0304
	200K	7.2279	4.6272	4.8227	-97.216	-18.997	6.4774	7.1772	-19.592	7.0967	1.0423
	300K	7.4682	4.5934	4.8398	-98.639	-18.864	6.3725	7.1981	-19.669	7.0967	1.0536
	400K	7.7252	4.5601	4.8578	-100.19	-18.737	6.2623	7.2192	-19.752	7.0967	1.0653
	500K	7.9890	4.5266	4.8763	-101.80	-18.612	6.1497	7.2405	-19.836	7.0967	1.0772

From Table-1, it is clear that the value of elastic constants at absolute zero are as per Cauchy,s relations,

$$C^0_{12} = C^0_{44},$$
$$C^0_{112} = C^0_{166},$$
$$C^0_{123} = C^0_{144} = C^0_{456}$$

These values are deviated on increase of temperature. This type of values are also found in other dielectric crystals [3, 16] . The mechanical properties like bulk modulus(B), anisotropic property(A), isotropic shear modulus(G), Young's modulus (Y) and Poisson's ratio(**ν**), toughness to fractor ratio (G/B) of the Os, OsC, OsN are presented on Table-2.

Table 2: Calculation of bulk Modulus(B in 10^{10}N/m^2), anisotropic ratio(A), shear Modulus(G in 10^{10}N/m^2), G/B ratio, Young Modulus(Y in 10^{10}N/m^2), Poisson ratio(ν), tetragonal moduli(C_S) and density(ρ in kg/m^3) of Os, OsC, OsN.

Material	Temp	B	A	G	G/B	Y	ν	Cs	ρ
Os	100K	7.9129	159.2038	2.4683	0.3120	6.7076	0.3587	5.0170	
	200 K	7.9901	36.7215	2.7100	0.3392	7.3042	0.3476	2.1824	
	300 K	8.0719	20.4539	2.949	0.3650	7.8870	0.3372	3.9318	22.23
	500K	8.2379	10.8366	3.3997	0.412	8.9658	0.3186	7.4736	
OsC	100K	5.6450	3.0938	3.0397	0.5385	7.7314	0.2717	1.5430	
	200 K	5.6732	2.8950	3.1280	0.5515	7.9270	0.2671	1.6534	16.5090
	300 K	5.731	2.6745	3.2381	0.564	8.1748	0.2623	1.7958	
	400K	5.7963	2.4741	3.3520	0.5783	8.4307	0.2576	1.9483	
	500K	5.8644	2.2983	3.4649	0.5910	8.6843	0.2532	2.1052	
OsN	100K	5.4603	4.0415	2.7655	0.5065	7.0981	0.2833	1.1899	
	200K	5.4941	3.7088	2.8642	0.5213	7.3206	0.2779	1.3003	
	300K	5.5517	7.5884	2.9824	0.5373	7.5884	0.2722	1.4374	16.64
	400K	5.6151	3.0696	3.1027	0.5527	7.8603	0.2667	1.5826	
	500K	5.6807	2.8167	3.2211	0.5672	8.1273	0.2616	1.7312	

The relative dielectricity of bonding in the material also has an important effect on it's hardness and can be determined by (G/B) ratio for Os, OsC, OsN ranges from 0.364 to 0.565, which are very close to those of OsB_2 (0.5) [17].
Table-2 depicts that Born stability criterion is also satisfied by these chosen materials i.e., $B = \dfrac{C_{11} + 2C_{12}}{3} \rangle 0, C_{44} \rangle 0$ and $C_S = \dfrac{C_{11} - C_{12}}{2} \rangle 0$

Where C_{11},C_{12} and C_{44} are SOECs.

Ultrasonic velocity is second one important parameter which can provide information about crystallographic texture. The ultrasonic velocity is related to elastic constant by following relation $v = \sqrt{\dfrac{C}{\rho}}$.

where C is the relevant elastic and ρ is the density of the particular material [18]. It can be seen by the Table-3 that ultrasonic velocity for longitudinal mode is found highest for OsC. We also observed that velocity for the shear mode along <100> and <110> are same for polarisation along <100> and $<1\bar{1}0>$ directions. This is due to the same formula along two different directions. This type of nature of velocity is similar to other materials like americium monopinictides [19].

Table 3: Ultrasonic velocities (in 10^3 m/s) of Os, OsC, OsN in temperature range (100K-500K) along different crystallographic directions.

Material	**Directions**	**Velocity**	**100K**	**200K**	**300K**	**400K**	**500K**
Os	<100>	V_L	1.8946	1.9301	1.9664	2.0025	2.0381
		$V_{S1}=V_{S2}$	1.8955	1.8987	1.9020	1.9054	1.9087
	<110>	V_L	2.6758	2.6893	2.7033	2.7174	2.7315
		V_{S1}	1.8955	1.8987	1.9020	1.9054	1.9087
		V_{S2}	2.1246	0.4431	0.5947	0.7160	0.8199
	<111>	V_L	2.8897	2.8985	2.9077	2.9170	2.9263
		V_{S1}	1.1012	1.1257	2.7033	1.1752	1.1994
		V_{S2}	1.1012	1.1257	1.1506	1.1752	1.1994
OsC	<100>	V_L	2.160	2.1844	2.2185	2.2549	2.2918
		$V_{S1}=V_{S2}$	1.7005	1.7027	1.7056	1.7088	1.7119
	<110>	V_L	2.5734	2.5825	2.5968	2.6123	2.6283
		V_{S1}	1.7005	1.7027	1.7056	1.7088	1.7119
		V_{S2}	1.3672	1.4153	1.475	1.5363	1.5970
	<111>	V_L	2.6972	2.7023	2.7112	2.7211	2.7313
		$V_{S1}=V_{S2}$	1.2598	1.2783	1.3019	1.3267	1.3517
OsN	<100>	V_L	2.0579	2.0842	2.1185	2.1547	2.1911
		$V_{S1}=V_{S2}$	1.700	1.7024	1.7054	1.7086	1.7119
	<110>	V_L	2.5318	2.5418	2.5559	2.5712	2.5867
		V_{S1}	1.700	1.7024	1.7054	1.7086	1.7119
		V_{S2}	1.1959	1.2502	1.3174	1.3792	1.4425
	<111>	V_L	2.6711	2.677	2.686	2.6957	2.7058
		$V_{S1}=V_{S2}$	1.2000	1.2195	1.2431	1.2677	1.2924

UGPs play a significant role in the study of thermal properties of the materials. It is used to describe physical properties of the materials as thermal expansion, thermal conductivity and temperature variation of elastic constants. The values of UGPs are more or less as other NaCl type materials [14].

Table 4: Ultrasonic Grüneisen parameters at 300K.

Material	*Grüneisen Parameter*	*Temperature(300K)*
Ultrasonic longitudinal wave propagating along <100>		
Os	$<\gamma_j^i>$	-1.4526
	$<(\gamma_j^i)^2>$	27.6979
OsC	$<\gamma_j^i>$	-0.5465
	$<(\gamma_j^i)^2>$	2.7612
OsN	$<\gamma_j^i>$	-0.5822
	$<(\gamma_j^i)^2>$	3.1012
Ultrasonic shear wave propagating along <100> and polarised along<100> direction		
Os	$<\gamma_j^i>$	0.5184
	$<(\gamma_j^i)^2>$	5.4770
OsC	$<\gamma_j^i>$	0.0676
	$<(\gamma_j^i)^2>$	0.1841
OsN	$<\gamma_j^i>$	0.0793
	$<(\gamma_j^i)^2>$	0.2326
Ultrasonic longitudinal wave propagating along <110> direction		
Os	$<\gamma_j^i>$	-1.8143
	$<(\gamma_j^i)^2>$	25.7698
OsC	$<\gamma_j^i>$	-0.7921
	$<(\gamma_j^i)^2>$	2.3981
OsN	$<\gamma_j^i>$	-0.8305
	$<(\gamma_j^i)^2>$	2.7267
Ultrasonic shear wave propagating along <110> and polarised along<001> direction		
Os	$<\gamma_j^i>$	-0.3536
	$<(\gamma_j^i)^2>$	2.7933
OsC	$<\gamma_j^i>$	-0.0111
	$<(\gamma_j^i)^2>$	0.2584
OsN	$<\gamma_j^i>$	-0.0288
	$<(\gamma_j^i)^2>$	0.3018
Ultrasonic shear wave propagating along <110> and polarised along $<1\bar{1}0>$ direction		
Os	$<\gamma_j^i>$	-0.2443
	$<(\gamma_j^i)^2>$	2.0596
OsC	$<\gamma_j^i>$	-0.5443

	$<(\gamma_j^i)^2>$	1.9077
OsN	$<\gamma_j^i>$	-0.5289
	$<(\gamma_j^i)^2>$	1.7894
Ultrasonic longitudinal wave propagating along <111>		
Os	$<\gamma_j^i>$	-2.8257
	$<(\gamma_j^i)^2>$	99.0635
OsC	$<\gamma_j^i>$	-0.8441
	$<(\gamma_j^i)^2>$	4.1073
OsN	$<\gamma_j^i>$	-0.9161
	$<(\gamma_j^i)^2>$	5.2623
Ultrasonic shear wave propagating along <111> and polarised along $<1\bar{1}0>$ direction		
Os	$<\gamma_j^i>$	-0.2568
	$<(\gamma_j^i)^2>$	1.1794
OsC	$<\gamma_j^i>$	-0.0844
	$<(\gamma_j^i)^2>$	1.3783
OsN	$<\gamma_j^i>$	-0.0922
	$<(\gamma_j^i)^2>$	1.2980

4. Conclusion

Thus in the present study, a simple method is used to findout the SOECs and TOECs using Coulomb and Born-Mayer potential. The trend of SOECs is in the following way $C_{11} > C_{44} > C_{12}$, while for TOECs $C_{144} > C_{456} > C_{123} > C_{166} > C_{111}$. The achieved results of the materials are fulfilled Born criterion, deviation of Cauchy,s relation at higher temperature, and the ductile nature. It is found that OsC is more ductile than Os and OsN. Ultrasonic velocity found highest for OsC, so it will be more promising candidate than the others. The UGPs are more and more influenced by SOECs and TOECs. Obtained results are very useful for the mechanical applications of these materials.

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