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First principles study of ceramic materials (IVB group carbides) under ultrafast laser irradiation*

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Group IVB carbides have been applied in extreme aerospace environments as hard ceramic coatings; ZrC is being considered as a replacement for SiC in nuclear reactors. Therefore, a thorough understanding of the laser irradiation response of group IVB carbides is of clear significance. However, the existing knowledge on the fundamental properties of IVB group carbides is limited and insufficient with regard to both irradiated and non-irradiated characteristics. We investigate the effect of ultrafast laser irradiation on the lattice stability of ceramic materials (IVB group carbides) using the density functional perturbation theory (DFPT). The calculated phonon frequencies of TiC and ZrC at the ground state are in good agreement with previous calculations and experimental values. The phonon frequencies of IVB group carbides are positive, even though the electronic temperature reached 5 eV. Thus, IVB group carbides are more stable under ultrafast laser irradiation, which has greater benefits in nuclear and aeronautical applications compared to metals (W, Na), semimetals (Bi), and semiconductors (Si, SiC). The thermodynamic properties of ZrC are calculated as functions of their lattice temperature at different electronic temperatures. The elastic shear constants of IVB group carbides satisfy the Born stability criteria at $T_e = 5$ eV. In addition, a comparison of the predicted melting temperatures of IVB group carbides, reveal that HfC is better suited for extreme high-temperature environments.

Keywords: first principle, lattice stability, elastic properties, electronic excitation

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1. Introduction

Ceramic materials (IVB group carbides) constitute different degrees of the three characteristic bonding forms: ionic, covalent, and metallic. These materials show good corrosion/oxidation resistance, very high melting point, extreme hardness, and other covalent properties. In addition, they exhibit strikingly high electrical/thermal conductivities compared with those of pure transition metals. Moreover, they have a NaCl-type structure that is associated with ionic bonding.[1–5] By exploiting their favorable physical and chemical properties, on the one hand, the transition metal carbide refractory ceramics can be candidate materials for use in high-temperature nuclear applications. In particular, ZrC is being considered as a coating material for the tri-isotropic coated nuclear fuel used in high temperature reactors, replacing or in addition to the currently used SiC.[6–8] Shen *et al.*[9] studied the lattice stability of β-SiC under ultrafast intense laser irradiation. To the best of our knowledge, there are no published reports on ZrC. On the other hand, transition metal carbides have numerous applications in the aeronautical industry.[10] Amir *et al.*[11] reported that the utilization of ceramic engine for the future aerospace applications may result in enhanced performance characteristics and reduced operational costs. Structural materials are typically exposed to various types of irradiation, including ultrafast particle and laser irradiation, in both nuclear applications and the aeronautical industry. The effects of fast neutron irradiation ($1 - 10 \times 10^{25}$ N/m^2 and 635–1480 °C) on the properties of high-purity zone refined zirconium carbide were measured by Snead *et al.*,[12] including the lattice parameter, hardness, elastic modulus, thermal conductivity, and indentation fracture toughness. They discovered that this ceramic is quite stable under fast neutron irradiation in the temperature and dose range. The processes of damage evolution in TiC crystals irradiated with hydrogen and deuterium ions at low temperatures were examined in situ with an electron microscope equipped with an ionic accelerator. Amorphization was confirmed upon hydrogen ion irradiation, while no amorphization occurred during deuterium ion irradiation.[13] The results of a previous study on the effect of ion irradiation on the microstructure stability of GFR ceramics (ZrC, ZrN, TiC, TiN, and SiC irradiated with 1 MeV Kr-Ions to 10 and 70 dpa at 800 °C) was reported.[14] Huang *et al.*[15] published results on the damage evolution of ZrC_X (where x ranges from 0.9 to 1.2) under proton irradiation at 800 °C, and discussed the irradiation-induced defects, such as density of dislocation loops, at different stoichiometries and

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doses. Changes in the physical properties under a range of irradiation and high temperature conditions are very important in nuclear and aeronautical applications. However, previously reported results on laser irradiation research on transition metal carbide refractory ceramics are limited to microsecond laser pulse interactions. There are few published calculations and experiments which specially focus on the effect of femtoseconds ultrafast intense laser irradiation on IVB group carbides.

Irradiating a target material using an ultrafast laser pulse ($\sim$ 100 fs) can excite a large number of electrons from the valence band to the conduction band. The electron-electron collisions result in the electronic energies approaching a Fermi-Dirac distribution with a well-defined electronic temperature T_e of approximately 10^4 K in a few tens of femtoseconds. However, the ion subsystem remains close to its initial temperature. Such a high electronic temperature would dramatically change the electronic charge distribution and the interatomic potential, inducing different physical effects on the target materials, such as phonon squeezing,[16] solid-solid transitions,[17–20] and non-thermal melting.[21–23] Herein, we perform calculations for the lattice dynamic, thermodynamic and elastic properties, and the predicted melting temperatures of IVB group carbides at different electronic temperatures.

The present investigation is organized as follows. In section 2, the computational method and technical details are described. Section 3 discusses the lattice dynamic, thermodynamic and elastic properties, and the predicted melting temperatures of IVB group carbides at different electronic temperatures. Finally, conclusions are summarized in Section 4.

2. Computational method and technical details

The calculations were performed with the Vienna *ab initio* simulation package (VASP) code[24–26] based on density functional theory (DFT). The projector-augmented wave (PAW)[27] method was employed to describe the electron-ion interactions. For all the geometrical optimizations and the calculations of properties, we adopted a face-centered cubic (fcc, space group $Fm\bar{3}m$, 225) structure. The exchange–correlation effects are mainly taken into account using the Perdew–Burke–Ernzerhof (PBE) function[28] of the generalized gradient approximation (GGA).[29] For TiC, ZrC, and HfC, the valence electrons configurations are $3d^24s^2$ for Ti, $4d^25s^2$ for Zr, $5d^26s^2$ for Hf, and $2s^22p^2$ for C, while the more tightly bound electrons are represented as core electrons. The plane-wave basis sets with the energy cutoff are set to 700 eV for TiC and 500 eV for ZrC and HfC. An $18\times18\times18$ Monkhorst–Pack mesh of k points in the first Brillouin zone (BZ) was sampled for geometrical optimization at the different electronic temperatures. All parameters were tested for convergence. Moreover, suitable bands were employed to ensure the availability of enough states for electrons to occupy even at high electronic temperatures.

Phonon frequencies were obtained by inter-atomic force constants in the real space[30,31] within density functional perturbation theory (DFPT)[32] at different electronic temperatures. In the calculation, we use the $2\times2\times2$ supercell and the $6\times6\times6k$ mesh to acquire the real space force constants. In addition, the thermodynamic functions (such as the phonon free energy F, the phonon internal energy E, the phonon entropy S, and the phonon heat capacity C_V) can be calculated from the phonon frequencies $w=(q,l)$ and phonon density of states $g(w)$ through the following functions.[32–34]

$$F = 3nN\int_0^{w_L} k_{\mathrm{B}}T\ln\left\{2\sinh\frac{hw}{4\pi k_{\mathrm{B}}T}\right\}g(w)\,\mathrm{d}w, \tag{1}$$

$$E = 3nN\int_0^{w_L}\frac{h}{4\pi}w\coth\left(\frac{hw}{4\pi k_{\mathrm{B}}T}\right)g(w)\,\mathrm{d}w, \tag{2}$$

$$C_V = 3nN\int_0^{w_L} k_{\mathrm{B}}\left(\frac{hw}{4\pi k_{\mathrm{B}}T}\right)^2\mathrm{csc}\,h^2\left(\frac{hw}{4\pi k_{\mathrm{B}}T}\right)g(w)\,\mathrm{d}w, \tag{3}$$

$$S = 3nN\int_0^{w_L} k_{\mathrm{B}}\left[\frac{hw}{4\pi k_{\mathrm{B}}T}\coth\left(\frac{hw}{4\pi k_{\mathrm{B}}T}\right) - \ln\left\{2\sinh\frac{hw}{4\pi k_{\mathrm{B}}T}\right\}\right]g(w)\,\mathrm{d}w, \tag{4}$$

where N is the number of primitive unit cells, n the number of atoms per primitive unit, h the Planck constant, k_{B} the Boltzmann constant.

At the same time, the total elastic moduli matrix was studied using the stress-strain method based on DFT with the $4\times4\times4k$ mesh. For cubic crystals, the Voigt average shear modulus $G=(3C_{44}+2C')/5$ was used to analyze the elastic stability of the structure, where C_{44} and $C'=(C_{11}-C_{12})/2$ are the two shear moduli.[35] From the results of the elastic moduli, the Debye temperature Θ_{D} at different electronic temperatures can be estimated using the following equation[36]

$$\theta_{\mathrm{D}} = \frac{h}{k_{\mathrm{B}}}\left[\frac{3n}{4\pi}\left(\frac{N_{\mathrm{A}}\rho}{M}\right)\right]^{1/3}v_m, \tag{5}$$

where v_m is the velocity of sound, k the Boltzmann constant, ρ the density, M the molecular weight, N_{A} the Avogadro number, and n the number of atoms in the molecule. The relationship between the Debye temperature Θ_{D} and the melting temperature T_{m} is assumed by the Lindermann melting criterion:[37] $T_{\mathrm{m}}=A\theta_{\mathrm{D}}^2$, where A depends on the density and the atom mass. We can therefore predict the melting temperature at different electronic temperatures utilizing the following relation: $T_{\mathrm{m}}/T_{\mathrm{m0}}=(\theta_{\mathrm{D}}/\theta_{\mathrm{D0}})^2$.

3. Results and discussion

3.1. Lattice optimization at different electronic temperatures

In order to investigate the effect of ultrafast laser irradiation on the lattice parameters, we first calculated the lattice pa-

rameters for the ground state. The values of TiC, ZrC and HfC are 4.3375 Å, 4.7239 Å, and 4.647 Å, respectively, which are very close to the experimental values[38] of 4.332 Å, 4.692 Å, and 4.639 Å, respectively. A comparison with experimental data revealed an overestimation of the equilibrium lattice parameters by 0.01% for TiC, 0.06% for ZrC and 0.02% for HfC. These results are in agreement by GGA standards. We then added the different electronic temperatures for the systems and obtain the optimized lattice parameters of the IVB group carbides. Figure 1 shows that the lattice parameters of the IVB group carbides clearly increased with an elevation of the electronic temperature. In addition, both TiC and ZrC exhibit approximately the same trend. As is well known, the systems are in mechanical equilibrium in the ground state. However, with the elevation of the electronic temperature, the previous equilibrium of the systems is destroyed by the electronic excitation. The inter-atomic attractive interactive would be weakened while the repulsive interaction is almost not affected by the excited electrons. To achieve a new equilibrium, the lattice volume expands, namely, the lattice parameters increases with an increase in the electronic temperature.

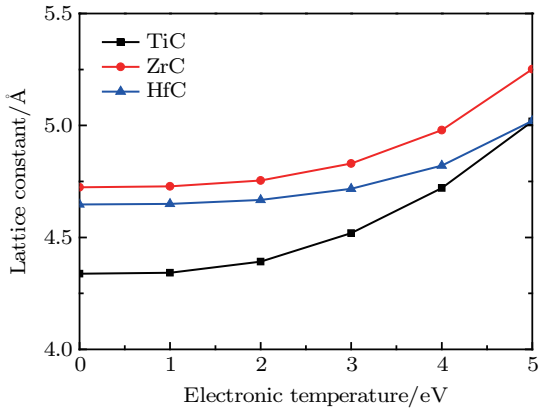


Fig. 1. (color online) The lattice parameters of IVB group carbides at different electronic temperatures.

3.2. Lattice dynamical properties at different electronic temperatures

We calculated the phonon dispersion curves of the IVB group carbides in fcc as a function of electronic temperature to investigate the lattice dynamic stability under ultrafast laser irradiation. The different imaginary phonon frequencies at some points of the Brillouin zone provided different information about lattice dynamic instability.[39] An imaginary frequency of the whole transverse acoustic branch at a high electronic temperature indicates a non-thermal melting transition.[40] An imaginary frequency of the whole longitudinal optical branch at the Γ point of the Brillouin zone indicates coherent optical phonon generation.[41] An imaginary frequency of a branch in the whole Brillouin zone is attributed to disordering of the lattice.[39]

Table 1. The calculated phonon frequencies (cm^{-1}) of TiC and ZrC at ground state and their comparisons with experimental and other theoretical values.

Location	Phonon mode	TiC/ZrC
Γ		15.93 (16.12[a], 15.81[c]) /13.14 (12.94[b], 12.95[c])
X	TA	8.51 (8.68[a], 8.53[c])/6.24 (6.28[b], 6.23[c])
	LA	10.66 (10.72[a], 10.74[c])/7.84 (7.99[b], 7.93[c])
	TO	15.93 (16.49[a], 15.60[c])/14.12 (14.16[b], 14.00[c])
	LO	17.83 (18.48[a], 17.72[c])/16.20 (17.13[b], 16.23[c])
L	TA	7.72 (8.06[a], 7.67[c])/5.47 (5.53[b], 5.39[c])
	LA	13.36 (13.32[a], 13.59[c])/9.76 (9.79[b], 9.68[c])
	TO	17.22 (17.09[a], 17.21[c])/15.76 (15.87[b], 15.66[c])
	LO	21.63 (21.63[a], 21.72[c])/19.91 (20.26[b], 19.86[c])

[a]Ref. [42], [b]Ref. [43], [c]Ref. [44]

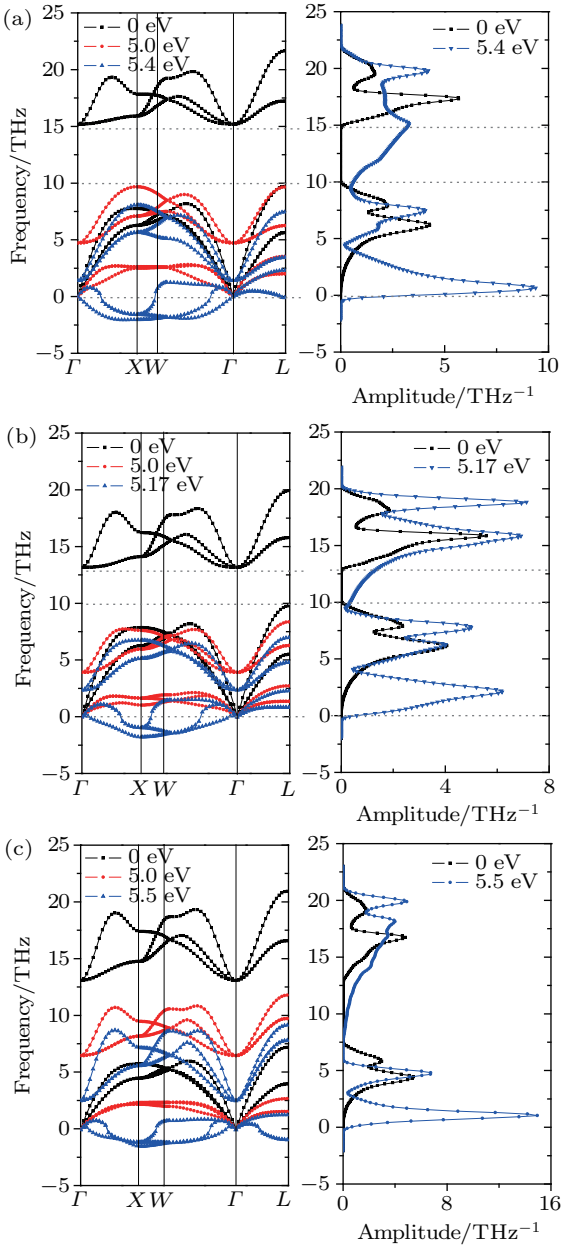


Fig. 2. (color online) The phonon spectra of (a) TiC, (b) ZrC, and (c) HfC obtained as a function of electronic temperature Te.

In Table 1, our calculated values of phonon frequencies at several high-symmetry points (Γ, X, and L) of the Brillouin

zone of TiC and ZrC at ground state are shown and compared with previous experimental[42,43] and theoretical values.[44] From Table 1, we can see that our calculated values are in excellent agreement with previous published experimental and theoretical data. This suggest that our results are reliable for the further studies at high electronic temperatures.

The phonon dispersion curves at different electronic temperatures are represented in Fig. 2. The optical and acoustic branches of the phonon spectrum of IVB group carbides holistically decreased with the elevation of the electronic temperature. Partial phonon frequencies begin to include imaginary frequencies, which signify the instability of the lattice at $T_e = 5.4$ eV for TiC, $T_e = 5.17$ eV for ZrC and $T_e = 5.5$ eV for HfC. It is noteworthy that even though the electronic temperatures reached 5.0 eV, the phonon frequencies of the IVB group carbides were positive. Thus the IVB group carbides have a higher stability under ultrafast laser irradiation, compared to metal (W, Na), semimetal (Bi) and semiconductor (Si, SiC).[9,35] All three of these become unstable in the electronic temperature range from 1.2 eV to 3.39 eV. The band gaps of the phonon density of states are 4.5801 THz, 2.624 THz, and 4.4339 THz for TiC, ZrC, and HfC at the ground state, respectively. Nevertheless, the phonon bands disappear at $T_e = 5.4$ eV for TiC and $T_e = 5.17$ eV for ZrC, and the phonon bands decrease to 1.3496 THz at $T_e = 5.5$ eV for HfC.

3.3. Thermodynamic properties at different electronic temperatures

Based on the phonon frequencies and phonon density of states, we investigated the thermodynamic properties (the phonon free energy F in Fig. 3, the phonon internal energy E in Fig. 4, the phonon entropy S in Fig. 5, and the phonon heat capacity C_V in Fig. 6) of ZrC at different electronic temperatures. These results provide reliable data for further theoretical and experimental studies on the relevant properties of the transition metal carbides. In Fig. 3, we can see that the phonon free energies increase as the lattice temperature is elevated. Furthermore, the phonon free energy–lattice temperature curves shift uniformly down with an increase in the electronic temperature. From $T_e = 0$ eV to 1 eV the relationship between the phonon free energy and the electronic temperature is almost unchanged. The F–T curves move down gradually with the elevation of the electronic temperature. Figure 4 indicates that the electronic excitation negatively affects the phonon internal energy of ZrC when the lattice temperature is relatively low. However, the discrepancies of the phonon internal energy among the different electronic temperatures are not obvious, as the lattice temperature increases.

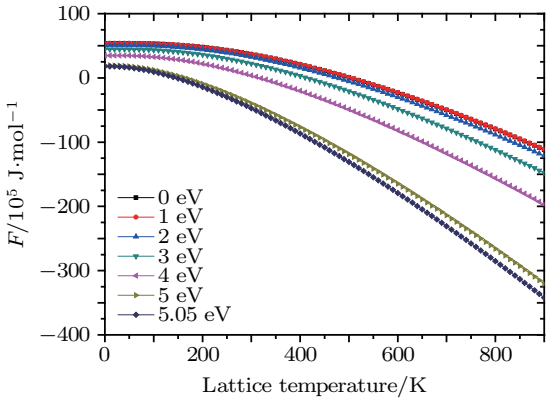


Fig. 3. (color online) The phonon free energy F of ZrC at different electronic temperatures.

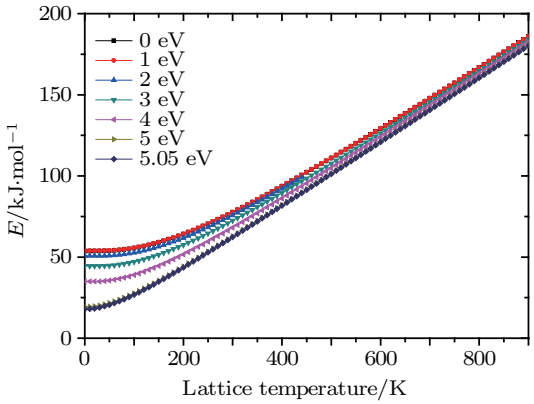


Fig. 4. (color online) The phonon internal energy E of ZrC at different electronic temperatures.

The phonon entropies corresponding to the lattice temperatures are provided in Fig. 5 for various electronic temperatures. It can be seen that the phonon entropy S increases with the elevation of the lattice temperature at different electronic temperatures. The electronic excitation positively affects the phonon entropy S at the same lattice temperature, which confirms that the randomness of ZrC increases as the effect of electronic excitation is enhanced. It is noteworthy that the phonon entropy-temperature curves exhibit a jump-change between $T_e = 4$ eV to 5 eV. Feng *et al.* proposed that such an abrupt change may be an indication of the target materials undergoing a phase transition, because of the imaginary transverse acoustic phonon frequencies in the jump-change.[45] However, there are no imaginary frequencies between $T_e = 4$ eV to 5 eV in Fig. 2. Therefore, the viewpoint of Feng *et al.* is not suited to our calculations. We consider that the difference is associated with the characteristic bonding forms of ZrC.

The phonon heat capacity C_V curves are provided in Fig. 6 at different electronic temperatures. At the low lattice temperature (less than 400 K), the effects of ultrafast laser irradiation on the phonon heat capacity are distinct. When the lattice temperature is larger than 900 K, the influence of ultrafast laser irradiation can essentially be neglected.

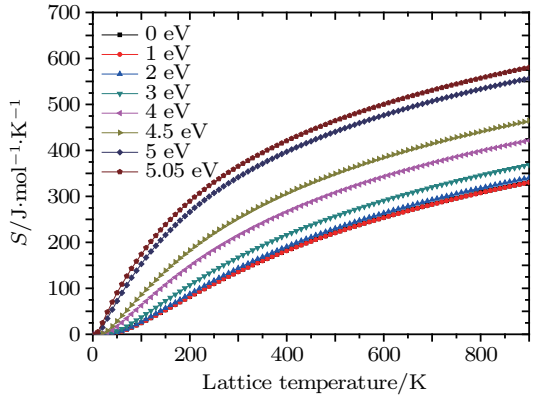


Fig. 5. (color online) The entropy S of ZrC at different electronic temperatures.

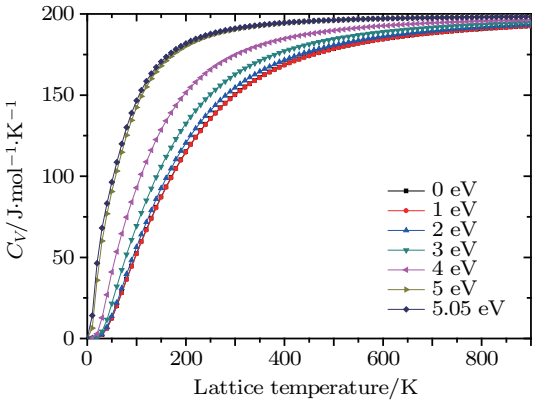


Fig. 6. (color online) The phonon heat capacity C_V of ZrC at different electronic temperatures.

3.4. Elastic properties and the melting temperatures at different electronic temperatures

The elastic properties of a lattice are directly described by the elastic constants C_{ij}. For the cubic lattice, there are three independent elastic constants (C_{11}, C_{12}, and C_{44}).

It is possible to show that a cubic lattice is dynamically stable if $B > 0$, $C' > 0$, and $C_{44} > 0$, criteria called the Born stability criteria. We defined the bulk modulus as $B = (C_{11} + 2C_{12})/3$ and the elastic shear constant $C' = (C_{11} - C_{12})/2$.[41] The computed quantities of elastic modulus and melting temperature T_m of TiC in Figs. 7(a) and 7(b), ZrC in Figs. 7(c) and 7(d) and HfC in Figs. 7(e) and 7(f) at different electronic temperatures are exhibited. We can see that both TiC and ZrC have approximately the same decreasing trends, except that the values are almost unchanged from $T_e = 0$ eV to 1 eV. HfC obviously moves down until the electronic temperature reaches 4 eV. The elastic shear constants of the IVB group carbides satisfy the Born stability criteria at $T_e = 5$ eV, which indicate the stability of the crystal for IVB group carbides.

When the target materials are in the ground state, the Debye temperatures of 920 K for TiC, 705 K for ZrC, and 547 K for HfC are close to the previously reported theoretical values of 935 K, 699 K, and 544 K.[46] The predicted melting temperatures of TiC decreased from 3340 K at the ground state to 1159 K at $T_e = 5$ eV. In addition, the predicted melting temperatures of ZrC exhibited a similar trend from 3698 K at the ground state to 1415 K at $T_e = 5$ eV. Finally, the predicted melting temperatures of HfC decreased from 4201 K to 2241 K, but these values are almost unchanged from $T_e = 0$ eV to 4 eV. The Debye temperatures of the IVB group carbides decreased at the ground state as the atomic number of the IVB group increased, but the melting temperatures reveal an inverse trend. The predicted melting temperatures of the IVB group carbides decreased as the electronic temperature increased. Particularly, the predicted melting temperatures of HfC are higher than TiC and ZrC at different electronic temperatures. Therefore, the use of HfC is advantageous in extreme high temperature environments.

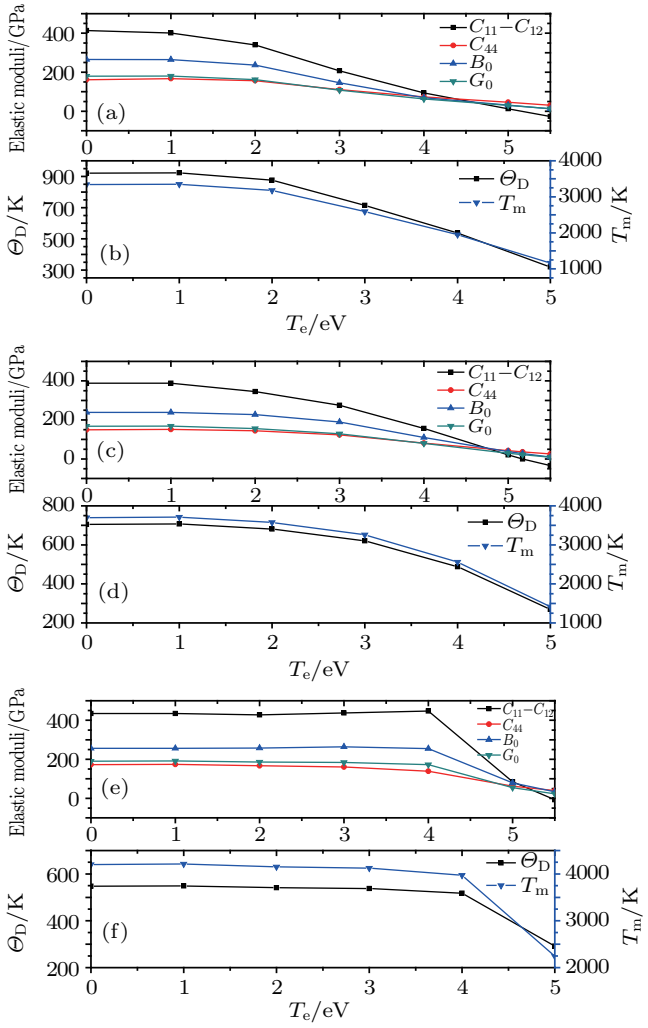


Fig. 7. (color online) Electronic temperature-dependent elastic moduli, Debye temperature Θ_D, and melting temperature T_m in (a) and (b) TiC, (c) and (d) ZrC, and (e) and (f) HfC.

4. Conclusion

In the present work, the effect of ultrafast laser irradiation on the lattice stability of ceramic materials (IVB group carbides) was investigated using density functional theory (DFT). The lattice parameters at different electronic temperatures for

the different structures were calculated and the values of the lattice parameter for the ground state are in excellent agreement with experimental values. Phonon frequencies were obtained using inter-atomic force constants in the real space within DFPT at different electronic temperatures. The calculated phonon frequencies of TiC and ZrC for the ground state show good agreement with previously reported calculations and experimental values. The phonon frequencies of the IVB group carbides are positive even though the electronic temperature peaked at 5.0 eV. Thus IVB group carbides are more stable under ultrafast laser irradiation compared to the metal (W, Na), semimetal (Bi) and semiconductor (Si, SiC), which is a beneficial property for nuclear and aeronautical applications. The thermodynamic properties of ZrC were calculated as a function of temperature for different electronic temperatures. We demonstrated that the elastic shear constants of the IVB group carbides satisfy the Born stability criteria at $T_e = 5$ eV, which indicate the stability of the crystal for IVB group carbides. The Debye temperatures of the IVB group carbides decreased at the ground state as the atomic number of the group increased, but the melting temperatures exhibited an inverse trend. In addition, a comparison of the predicted melting temperature of the IVB group carbides revealed that HfC is best suited for extreme high temperature environment applications.

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