# Mean-field potential calculations of shock-compressed porous carbon

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(Received 3 September 2004; revised manuscript received 1 December 2004; published 22 February 2005)

The mean-field potential approach with first-principles total energy data as input is used to investigate shock-compressed carbon with initial densities of 3.51, 2.2, 1.85, and 1.6 $g/cm^3$ up to 1400 GPa. We have calculated the shock Hugoniot, and the temperature and electronic contribution to the heat capacity along the Hugoniot. While excellent agreement with underground nuclear explosion data is obtained, our results do not show the high compressibility of carbon at megabar pressures indicated by recent laser-driven shock wave experiments.

DOI: 10.1103/PhysRevB.71.054110 PACS number(s): 64.10.+h, 71.15.Nc, 05.10.−a, 05.70.Ce

## I. INTRODUCTION

The equation of state (EOS) of carbon has recently been investigated both experimentally and theoretically.[1–5] Very recently, Batani *et al.* carried out laser-driven shock wave studies of the EOS of porous carbon[1] and found that their measured shock Hugoniot points for two different initial densities of carbon fell below the Hugoniot derived from the SESAME tables.[6] They pointed out that, despite the large error bars, the systematic deviation of their data from the theoretical curve indicates that the compressibility of carbon is greater than theoretical predictions, but they admit that this discrepancy may be due to systematic errors in their experimental technique. We note that EOS data on deuterium from laser-driven shock wave experiments[7–10] show significant departures from the SESAME model (see Knudson *et al.*[11]), *ab initio* calculations,[12–15] and other experiments.[11,16] While Ross and Yang[17] attributed the discrepancy to the failure of the current implementation of density functional theory, Nellis[18] suggested that the laser-driven shock wave results were incorrect.

If limited to the solid state, the high-pressure EOS of carbon can be reliably calculated in the quasiharmonic approximation with the phonon contribution evaluated using density functional perturbation theory.[3,19] However, the traditional Debye-Grüneisen method[2,20] is the most widely used approach (it is used to construct the SEASAME EOS tables) but it is not only limited to solids, but also depends on the modeled density dependence of the Grüneisen parameter ($\gamma$), such as $\gamma\rho=$const ($\rho$ is the density). In this paper we calculate the Hugoniots of carbon with initial densities of 3.51, 2.2, 1.85, and 1.6 $g/cm^3$ up to 1400 GPa using the mean-field potential (MFP) approach,[21–26] which has been tested for many elemental materials, including porous solids.[27] Variations in the initial density allow us to study more of the EOS surface of carbon. (Since the MFP method incorporates the one-particle mean-field model, it is not possible to study molecular liquid deuterium without first extending the technique.)

## II. THEORETICAL METHOD

We first give a brief summary of the MFP approach. In a couple of papers,[21,22] the classical MFP approach was developed to calculate the various thermodynamic quantities of metals. The MFP approach was first tested on the metal Ce.[21] The transition pressure and volume change of the well known $\gamma$-$\alpha$ isostructural transition at 300 K, the experimental Hugoniot, and the 300 K isotherm were well reproduced. The MFP approach was then checked for the five metals Al, Cu, Ta, Mo, and W.[22] The calculated Hugoniots and 293 K isotherms fell well within the experimental uncertainties. The MFP yields Hugoniots for porous copper, nickel, and molybdenum in good agreement with experiment, including cases of anomalous compressibility.[27]

Let us consider a system with a given averaged atomic volume $V$ and temperature $T$. It is known that the vibrational contribution to the partition function takes the form $Z_{\rm ion}=\exp(-NF_{\rm ion}/k_BT)$, where $N$ is the total number of lattice ions and $F_{\rm ion}$ is the vibrational free energy of an ion. In the mean-field approximation, the classical $Z_{\rm ion}$ is given by

$$Z_{\rm ion}=\left(\frac{Mk_BT}{2\pi\hbar^2}\right)^{3N/2}\{\int \exp[-g(\mathbf{r},V)/k_BT]d\mathbf{r}\}^N. \qquad (1)$$

The essential feature of the MFP approach is that the mean-field potential $g(\mathbf{r},V)$, is simply constructed only in terms of the 0-K total energy $E_c$, which is obtained from *ab initio* electronic structure calculations

$$g(r,V)=\frac{1}{2}[E_c(R+r)+E_c(R-r)-2E_c(R)]. \qquad (2)$$

It has been shown[21] that the well-known Dugdale-MacDonald[28] expression for the Grüneisen parameter can be derived by expanding $g(r,V)$ to order $r^2$.

As a result, when the magnetic contribution is neglected, the Helmholtz free energy per ion $F(V,T)$, can be written as the sum of the cold ($T=0$), vibrational ionic, and thermal electronic contributions

 

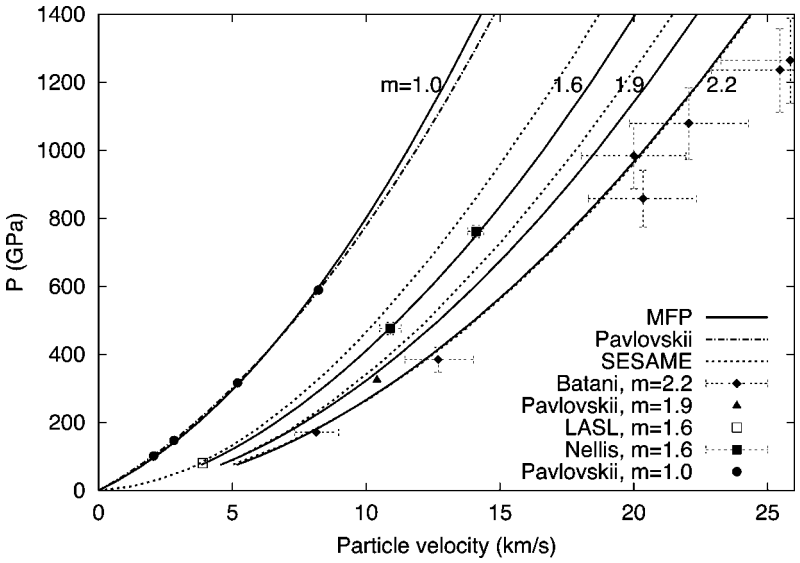


FIG. 1. Hugoniot pressure versus particle velocity of diamond for initial porosities $m=1.0$, 1.6, 1.9, and 2.2. The solid lines represent the results of the present calculation. The dot-dashed line at $m=1.0$ is the empirical fit $u_s=12.16+1.00u_p$ of Pavlovskii (Ref. 35); and the dotted lines at $m=1.57$ ($\rho_0=2.23$ g/cm$^3$), $m=1.9$ ($\rho_0=1.85$ g/cm$^3$), and 2.2 ($\rho_0=1.6$ g/cm$^3$) were obtained by Batani *et al.* (Ref. 1) from the SESAME tables. The data points are ●: Pavlovskii (Ref. 35), □: LASL (Ref. 36), ■: Nellis (Ref. 2), ▲: Pavlovskii *et al.* (Ref. 34), and ◆; Batani *et al.* (Ref. 1).

$$F(V,T) = E_c(V) + F_{\text{ion}}(V,T) + F_{\text{el}}(V,T), \tag{3}$$

$$F_{\text{ion}}(V,T) = -k_B T\left(\frac{3}{2}\ln\frac{mk_BT}{2\pi\hbar^2} + \ln\,\nu_f(V,T)\right), \tag{4}$$

$$\nu_f(V,T) = 4\pi\int \exp\left(-\frac{g(r,V)}{k_BT}\right)r^2dr, \tag{5}$$

$$F_{\text{el}} = E_{\text{el}} - TS_{\text{el}}, \tag{6}$$

$$E_{\text{el}}(V,T) = \int n(\varepsilon,V)f\varepsilon d\varepsilon - \int^{\varepsilon_F} n(\varepsilon,V)\varepsilon d\varepsilon, \tag{7}$$

$$S_{\text{el}}(V,T) = -k_B\int n(\varepsilon,V)[f\ln f + (1-f)\ln(1-f)]d\varepsilon. \tag{8}$$

In the above equations, $F_{\text{ion}}$ is the ionic vibrational free energy, $F_{\text{el}}$ is the free energy due to the thermal excitation of electrons, $n(\varepsilon,V)$ is the electronic density of states (DOS), $f$ is the Fermi distribution, and $\varepsilon_F$ is the electronic Fermi energy.

Other thermodynamic functions can be obtained in the usual way from $F(V,T)$; specifically, entropy is $S=-(\partial F/\partial T)_V$, internal energy is $E=F+TS$, pressure is $P=-(\partial F/\partial V)_T$, and the Gibbs free energy is $G=F+PV$.

## III. COMPUTATIONAL DETAILS

The $P$-$V$ Hugoniot was obtained from the Rankine-Hugoniot relation $P(V_0^{\text{porous}}-V)/2=E-E_0^{\text{porous}}$, where $V_0^{\text{porous}}$ is initial specific volume and $E_0^{\text{porous}}$ is the initial specific internal energy. In all of our Hugoniot calculations we take the carbon structure to be that of diamond (3.51 g/cm$^3$ ambient density); hence, our initial densities of 2.2, 1.85, and 1.6 g/cm$^3$ correspond to "porous diamond." This is a reasonable approximation since the measured enthalpy difference between diamond and graphite under standard conditions is just −19 meV/atom (see Janotti *et al.*,[29] and references therein). The effect of this difference on the Hugoniot temperatures is less than 100 K, which is not discernable in the figures plotted in this paper. We only consider pressures above the graphite-diamond transformation pressure and assume the final states are completely compacted. In this case, it is a good approximation to take the initial specific energy $E_0^{\text{porous}}$ for porous carbon to be exactly the same as the initial specific energy $E_0$ for nonporous carbon. The initial volume of the porous material is $V_0^{\text{porous}}=m\,V_0$, where $m$ is the initial porosity and $V_0$ is the ambient volume of nonporous single-crystal diamond. Our initial densities of 3.51, 2.2, 1.85, and 1.6 g/cm$^3$ correspond to $m=1.0$, 1.6, 1.9, and 2.2, respectively.

Mitchell *et al.*[30] found that the effects of shock melting on the $P$-$V$ Hugoniots of several reference metals were too weak to be observed; hence we have neglected shock melting and the phase dependence of the high-temperature equation of state in our calculations of the carbon Hugoniots.

The 0-K total energy was calculated using the full-potential linearized augmented plane wave (LAPW) method[31,32] in the generalized gradient approximation (GGA).[33] To ensure continuity of the calculated energy as a function of volume, we used constant muffin-tin radii of $1.0a_0$ (Bohr radius). The input to all of our thermodynamic calculations consists of both LAPW-calculated energies and points obtained by cubic spline interpolation with nodes separated by $0.005a_0$. Outside the region where the LAPW calculations are applicable, Morse function extrapolations toward zero and infinity are used to complete the 0-K energy curve.

## IV. RESULTS AND DISCUSSION

### A. Pressure versus particle velocity

Laser-driven shock wave data are usually presented in the $u_p$-$P$ plane because of the large error bars on the measured densities. Our calculated results for $m=1.0$, 1.6, 1.9, and 2.2 are plotted in the $u_p$-$P$ plane in Fig. 1 together with experi-

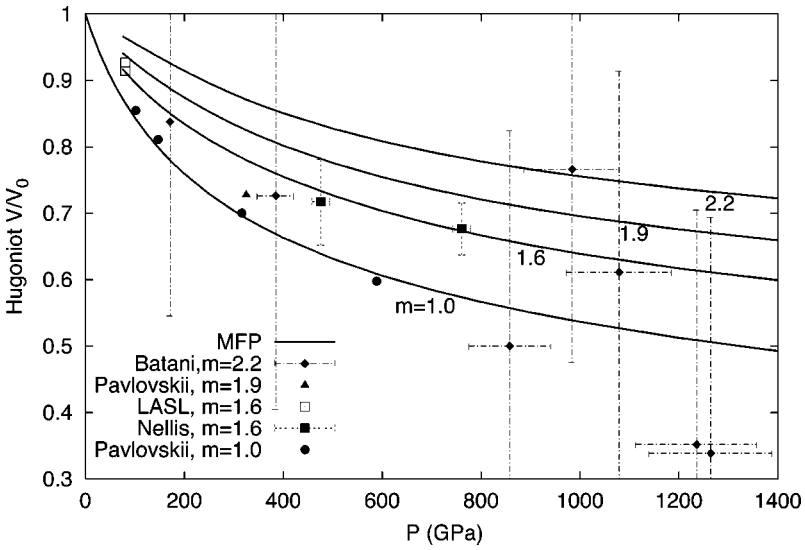


FIG. 2. Relative Hugoniot volume versus pressure for diamond with initial porosities $m=1.0$, 1.6, 1.9, and 2.2. $V_0$ is the ambient atomic volume of single-crystal diamond. The solid lines represent the results of the present calculation. The data points are ●: Pavlovskii (Ref. 35), ▲: Pavlovskii *et al.* (Ref. 34), □: LASL (Ref. 36), ■: Nellis (Ref. 2), and ◆: Batani *et al.* (Ref. 1).

mental data.[1,2,34–36] The porosity $m=1.0$ (initial density $=3.51$ g/cm$^3$) corresponds to single crystal diamond, and $m=1.6$ (initial density$=2.2$ g/cm$^3$) corresponds to pyrolytic graphite. For these two porosities, our calculated $u_p$-$P$ Hugoniots agree with the measurements[2,35,36] to within the experimental error bars. For $m=1.0$, we believe that the small but growing difference between the empirical fit $u_s=12.16+1.00u_p$ of Pavlovskii[35] and our calculations above 600 GPa is a consequence of extrapolating the fit to pressures above those of the data that were available to Pavlovskii ($P<600$ GPa). Nellis *et al.*[2] calculated the graphite Hugoniot by taking it to be "porous diamond" at $m=1.6$ and found that their theoretical curve deviated significantly from their measurements for $P>300$ GPa, but still our calculations show excellent agreement with their measurements. For $m=2.2$, the laser-driven shock wave results of Batani *et al.*[1] are systematically lower than our calculations at a given particle velocity, and they are also systematically lower than the Hugoniot obtained from the SESAME tables.

Figure 1 includes the SESAME Hugoniots for $m=1.6$, 1.9, and 2.2 obtained by Batani *et al.*[1] from the SESAME EOS of graphite ($m=1.6$). The Hugoniots for $m=1.6$ and 1.9 disagree with our MFP results, while the Hugoniot for $m=2.2$ is in close agreement. The discrepancy is most likely due to inaccuracy in the Grüneisen gamma used to construct the SESAME EOS.[37] The agreement between the MFP and SESAME Hugoniots for $m=2.2$ is fortuitous.

### B. Relative volume ($V/V_0$) versus pressure

In Fig. 2, a plot of $V/V_0$ versus $P$, the errors due to the uncertainties in the particle velocity measurements are enlarged enormously. Note that the errors in the relative volume for the laser-driven shock wave experiments by Batani *et al.*[1] for $m=2.2$ span the entire volume range from $m=1.0$ to $m=2.2$ at a given pressure.

For $m=1.9$ ($\rho_0=1.85$ g/cm$^3$), the relative volume measured by Pavlovskii *et al.*[34] at 325 GPa is 0.728. In contrast, our calculated relative volume is 0.825. The discrepancy between our calculation and the measurement by Pavlovskii *et al.*[34] for $m=1.9$ may be due to inaccuracy in their measurement. We can see from Fig. 2 that the graphite Hugoniot data[2,36] for $m=1.6$ ($\rho_0=2.2$ g/cm$^3$) show a trend toward a larger value of $V/V_0$ than 0.728 at 325 GPa. Note that the shock experiment of Pavlovskii *et al.*[34] on carbon for $\rho_0=1.85$ g/cm$^3$ ($m=1.9$) gives a density at 325 GPa that is higher than that obtained for $\rho_0=2.2$ g/cm$^3$ ($m=1.6$) from our MFP calculations at the same pressure, or by extrapolation of the data of Nellis *et al.*[2] to 325 GPa.

### C. Hugoniot temperatures

Our results for $m=1.0$, 1.6, 1.9, and 2.2 are plotted in the $T$-$V/V_0$ plane in Fig. 3(a), which also shows the carbon Hugoniot temperatures for $m=1.0$ and 1.847 calculated by Pavlovskii.[35] Our result for $m=1.0$ is in good agreement with that of Pavlovskii, while his result for $m=1.847$ is closer to our result for $m=1.6$ than to our result for $m=1.9$. It should be mentioned that standard temperature estimates are rather uncertain due to the shortage of data on the Grüneisen parameter and specific heat.

The calculated Hugoniot temperatures as a function of pressure up to 1400 GPa are listed in Table I and compared to the model results of Fried and Howard[4] (FH) in Fig. 3(b). At a given pressure the Hugoniot temperature increases with the porosity because of the larger volume collapse and the corresponding larger increase in internal energy. While very good agreement is obtained between our calculation and the FH modeling for $m=1.0$ (diamond) and $m=1.6$ (graphite), our calculated temperature for $m=1.9$ at 325 GPa is 21758 K, which is almost 50% higher than the 15000 K obtained by FH. FH obtained their EOS by generalizing the approximate Murnaghan functional form. The EOS parameter values were chosen to ensure agreement with two types of data: (1) accurate thermodynamic data, specifically the 300 K isotherms and temperature dependences of the heat capacities of both diamond and graphite, thus the good agreement between FH and MFP for the $m=1.0$ and $m=1.6$ Hugoniot temperatures; (2) inaccurate shock data, namely the measurement of Pavlovskii *et al.*[34] for $m=1.9$, which is

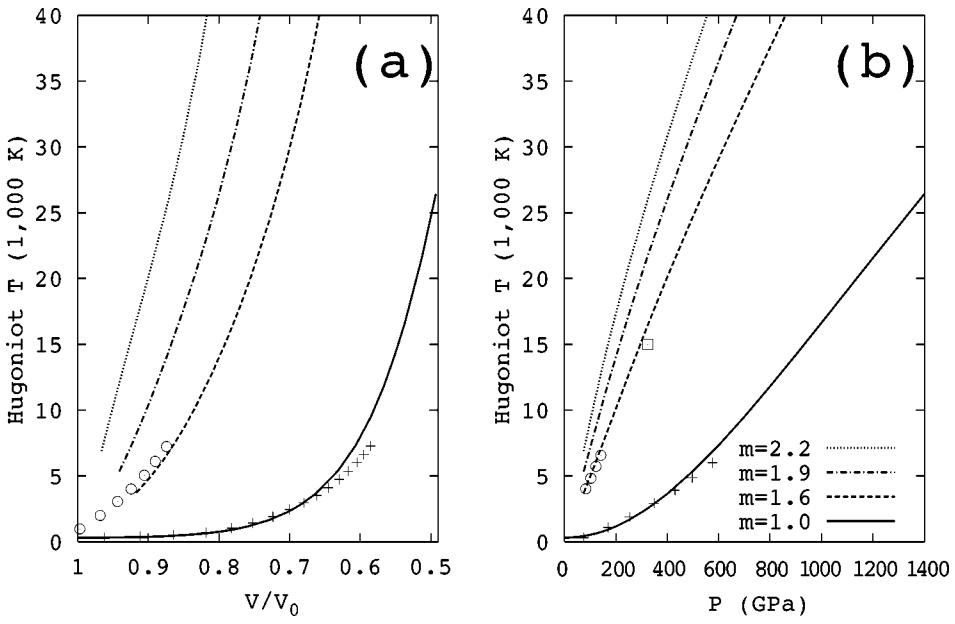


FIG. 3. Hugoniot temperatures for diamond with initial porosities $m=1.0$, 1.6, 1.9, and 2.2. The curves are the results of our MFP calculations. (a) Hugoniot temperature as a function of relative volume $V/V_0$. The points are Pavlovskii's (Ref. 35) for $m=1.0$(+) and 1.847 (○), (b) Hugoniot temperature versus pressure. Here the points are from Fried and Howard (Ref. 4): $m=1.0$(+), 1.6 (○), and 1.9 (□).

inconsistent with our MFP Hugoniot (see previous subsection), hence the discrepancy between the FH and MFP Hugoniot temperatures for $m=1.9$ at 325 GPa.

### D. Shock-induced insulator-conductor transition in carbon

The pressure-induced metallization of non-metals has been the subject of a number of theoretical and experimental studies.[38–41] At low temperatures, metallization is associated with the closing of the electronic band gap. We have calculated the electronic band gap of diamond-type carbon as a function of $V/V_0$; see Fig. 4(a). The calculated band gap increases with density, as also found by Surh *et al.*[39] and by Fahy and Louie.[40] This implies that diamond-type carbon becomes a more effective insulator with increasing hydrostatic pressure, in agreement with experiment.[41] This unusual

TABLE I. The calculated relative volume $V/V_0$ and temperature for diamond with initial porosities $m=1.0$, 1.6, 1.9, and 2.2. $V_0$ is the atomic volume of single-crystal diamond under ambient conditions.

| $m$ | 1.0 | | 1.6 | | 1.9 | | 2.2 | |
|---|---|---|---|---|---|---|---|---|
| $P$ (GPa) | $V/V_0$ | $T$ (K) | $V/V_0$ | $T$ (K) | $V/V_0$ | $T$ (K) | $V/V_0$ | $T$ (K) |
| 75 | 0.8726 | 429 | 0.9155 | 3707 | 0.9397 | 5328 | 0.9646 | 6881 |
| 100 | 0.8437 | 520 | 0.8952 | 4937 | 0.9242 | 7098 | 0.9538 | 9123 |
| 125 | 0.8185 | 637 | 0.8772 | 6201 | 0.9099 | 8875 | 0.9433 | 11307 |
| 150 | 0.7963 | 783 | 0.8609 | 7492 | 0.8967 | 10634 | 0.9328 | 13405 |
| 175 | 0.7768 | 960 | 0.8464 | 8797 | 0.8843 | 12356 | 0.9225 | 15411 |
| 200 | 0.7594 | 1165 | 0.8330 | 10106 | 0.8726 | 14032 | 0.9126 | 17333 |
| 250 | 0.7292 | 1649 | 0.8091 | 12705 | 0.8513 | 17244 | 0.8942 | 20967 |
| 300 | 0.7038 | 2229 | 0.7883 | 15244 | 0.8323 | 20288 | 0.8775 | 24387 |
| 325 | 0.6925 | 2552 | 0.7789 | 16487 | 0.8238 | 21758 | 0.8698 | 26035 |
| 350 | 0.6820 | 2897 | 0.7700 | 17711 | 0.8155 | 23197 | 0.8624 | 27649 |
| 400 | 0.6631 | 3647 | 0.7535 | 20105 | 0.8005 | 26000 | 0.8490 | 30792 |
| 500 | 0.6315 | 5367 | 0.7255 | 24708 | 0.7745 | 31366 | 0.8259 | 36823 |
| 600 | 0.6059 | 7338 | 0.7022 | 29119 | 0.7532 | 36504 | 0.8069 | 42612 |
| 700 | 0.5847 | 9507 | 0.6825 | 33389 | 0.7350 | 41481 | 0.7906 | 48230 |
| 800 | 0.5665 | 11818 | 0.6656 | 37553 | 0.7195 | 46336 | 0.7768 | 53719 |
| 900 | 0.5506 | 14215 | 0.6508 | 41633 | 0.7060 | 51094 | 0.7647 | 59106 |
| 1000 | 0.5366 | 16655 | 0.6379 | 45646 | 0.6944 | 55773 | 0.7540 | 64417 |
| 1200 | 0.5126 | 21565 | 0.6160 | 53510 | 0.6745 | 64954 | 0.7360 | 74882 |
| 1400 | 0.4927 | 26438 | 0.5981 | 61213 | 0.6584 | 73974 | 0.7211 | 85221 |

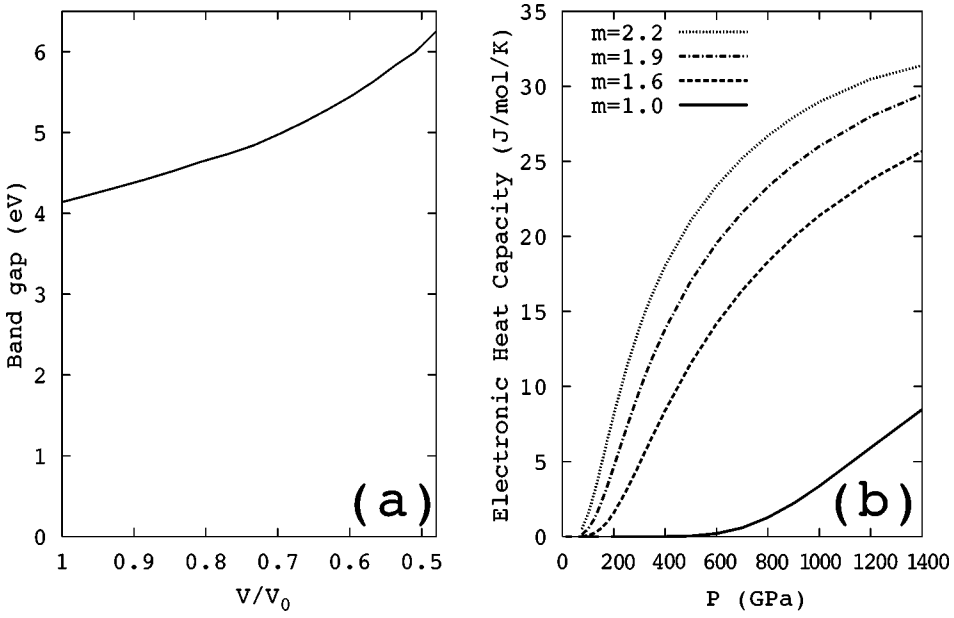


FIG. 4. (a) The calculated band gap of carbon as a function of relative volume $V/V_0$. (b) The calculated electronic heat capacity of diamond as a function of pressure for initial porosities $m=1.0$, 1.6, 1.9, and 2.2.

behavior is usually explained in terms of the splitting of bonding and antibonding $sp^3$ states of carbon.[39,41]

However, in the case of shock-wave compression, the increase in temperature along the Hugoniot must be taken into account, especially in the case of porous materials, which generate high temperatures during volume collapse (Fig. 3). High temperatures could excite electrons from the valence band to the conduction band of carbon, even though the band gap is very large. For $m=1.0$, 1.6, 1.9, and 2.2, we have also calculated the electronic contribution to the heat capacity $C_{\mathrm{el}}=dE_{\mathrm{el}}/dT$ [see Eq. (7) for the definition of $E_{\mathrm{el}}$], of carbon along its Hugoniot. An abrupt increase in $C_{\mathrm{el}}$ from zero in the low-pressure insulating state is an unambiguous signature for the insulator-conductor transition. In Fig. 4(b), we see that while single-crystal diamond does not become a conductor until shocked up to 600 GPa, diamond with a porosity of $m=2.2$ can be transformed into a conductor by shock loading to a pressure of approximately 80 GPa.

## V. SUMMARY

To summarize, the Hugoniots of carbon with porosities $m=1.0$, 1.6, 1.9, and 2.2, corresponding to initial densities of $\rho_0=3.51$, 2.2, 1.85, and 1.6 g/cm$^3$, respectively, have been calculated by the MFP approach. The present calculation shows excellent agreement with the underground nuclear explosion data[2,35] at $m=1.0$ (single-crystal diamond) and 1.6 (graphite). In contrast, our calculations do not show the high compressibility of carbon at megabar pressures observed by Batani *et al.*[1] in their very recent laser-driven shock wave experiment, nor do our MFP results support the measurement of Pavlovskii *et al.*[34] for $m=1.9$. In addition, we also studied the possible insulator-metal transition in shocked carbon. We found that single-crystal diamond will not transform into a metal until shocked up to 600 GPa, but porous diamond with $m=2.2$ is predicted to transform into a metallic state at $P=80$ GPa.

## ACKNOWLEDGMENT

This work was supported by the National Science Foundation through Grants No. DMR-9983532 and DMR-0122638. Calculations were carried out on the IBM-SP3 supported by the DOD High Performance Computer Modernization Program at the ASC-MSRC and the LION-XL cluster at Pennsylvania State University supported in part by NSF Grant No. DMR-0205232 and in part by the Materials Simulation Center led by Dr. Sofo at Pennsylvania State University. This work was also supported in part by the Swedish Foundation for Strategic Research (SSF), the Swedish Natural Science Research Council (NFR), and the Göran Gustafsson Foundation. Two of us (L.B., D.L.P.) wish to thank J.D. Johnson for very valuable discussions on the equation of state of carbon.

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