

D'yakov-Kontorovich instability of shock waves in hot plasmasNadine Wetta, Jean-Christophe Pain,^{*} and Olivier Heuzé
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The D'yakov-Kontorovich stability criterion for spontaneous emission of acoustic waves behind shock fronts is investigated for high-temperature carbon, aluminum, silicon, and niobium plasmas. The D'yakov and critical stability parameters are calculated along the principal Rankine-Hugoniot curve with an equation-of-state model in which the contribution of bound and free electrons is calculated through a relativistic quantum average-atom model, solving the Dirac equation. The pressure is determined using the stress-tensor formula in the relativistic framework. We find that the instability occurs at the end of the ionization of electronic shells, when the Hugoniot curve departs from the $\rho/\rho_0 = 4$ asymptote to tend to the $\rho/\rho_0 = 7$ limit. In such conditions, if the plasma is optically thick, the contribution of blackbody radiation to the EOS is dominant, and the system becomes always stable. Our results indicate that the conditions in which the instability takes place are different from previously published estimates, due to assumptions made in the corresponding equation-of-state models, especially as concerns the relativistic effects, and depend on the radiative opacity of the material.

DOI: [10.1103/PhysRevE.98.033205](https://doi.org/10.1103/PhysRevE.98.033205)**I. INTRODUCTION**

The large interest on the study of plasma instabilities is not only triggered by fundamental physics curiosity but stems from important plasma applications. Such instabilities are the result of any disturbance that may occur in a plasma parameter such as density, temperature, magnetic or electric field, or current. They dictate the plasma behavior and evolution [1]. Several theories predict that matter properties can lead to instabilities which can affect the well-known steady shock wave propagation scheme and cause major loss of efficiency in inertial confinement fusion (ICF) or misunderstanding of astrophysical phenomena [2–4]. Therefore, the experimental existence of these instabilities has to be investigated and their consequences mastered versus time and space. A first case of instability corresponds to the change of convexity of the equation of state [5–12]. It can be discontinuous like phase transitions which lead to split shocks (laboratory impact experiments), or continuous (plasma phase transitions [13,14] found, for instance, in neutron star collisions) which generates a combination of shocks and isentropic compressions [15,16]. A second case is called the D'yakov-Kontorovich instability [17,18]. Up to now no proof of its existence in the Universe has been found [19]. We study here the case of increasing pressure-volume relationship on the Hugoniot which is mainly obtained after the first ionization in plasmas. In a former study [20], we explored the equation of state in this domain for three metals (aluminum, iron and copper) of very different densities, but found no possibility of its existence. Our recent calculations at much higher temperature and pressure, taking into account relativistic effects, showed us a possibility to reach these conditions. It is the purpose of the present work.

The study of this instability in shock waves propagating in a medium has been a subject of research for many decades (see, for instance, Refs. [21–25]). It occurs from initial perturbations in the shock front, which may grow exponentially during the course of shock propagation, or arise from spontaneous emission of sound waves and entropy vortex waves [26] which take away energy from the shock wave, resulting in its decay. The first type may be reduced by minimizing initial perturbations in the system. The second kind, which has the form of a nonvanishing “flutter” on the surface of the shock wave without an increase or decrease of the perturbations, depends mainly on the material properties, in particular, thermodynamic conditions, i.e., on the equation of state (EOS). There are several experimental evidences of shock instability in ionizing and dissociating gases [27,28]. It would be worth investigating whether experimental evidence of shock instability or unexplained events could be associated to some theoretically predicted phenomena.

The conditions for the onset of instability in a medium with an arbitrary EOS were first derived by D'yakov [17] and Kontorovich [18]. It is known that the EOS of the material affects the stability criteria to a great extent. D'yakov's analysis was again re-examined by Fowles and Swan [29–32]. Interaction of small perturbations of the form $e^{i(kx-\omega t)}$ with the planar shock front yields the stability criteria first derived by D'yakov and Kontorovich. It provides the conditions for which spontaneous emission of sound occurs in the shock compressed material. When a sinusoidal perturbing wave is incident on the shock front, from the compressed side, a reflected wave is produced. This wave is likely to carry shock energy away from the front. To hold momentum and energy conservation across the shock front, an entropy vortex wave, characterized by zero pressure perturbation, is also produced along with the reflected sound wave, whose amplitude depends on the reflection coefficient, which is itself dependent on the Rankine-Hugoniot curve and the frequency of the incident sound wave. Spontaneous sound

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emission occurs when the amplitude of this reflected wave is finite in the limit of vanishing amplitude of the incident wave.

Let us consider the shocked state in the (P, V) (P being the pressure and V the volume) diagram and its related slopes associated to different curves:

(1) \mathcal{H} the slope of the Hugoniot curve:

$$\mathcal{H} = - \left. \frac{dP}{dV} \right|_{\mathcal{H}}, \quad (1)$$

the subscript \mathcal{H} meaning “along the Hugoniot shock adiabat”,

(2) \mathcal{R} the slope of the Rayleigh line:

$$\mathcal{R} = \frac{P - P_0}{V_0 - V} = j^2, \quad (2)$$

where $j = \rho_0 D = \rho(D - u)$ is the mass flow (ρ being the matter density), D and u being the shock and material velocities respectively, and 0 denotes the initial state (pole).

(3) S the slope of the isentropic curve:

$$S = - \left. \frac{\partial P}{\partial V} \right|_S = \frac{c_s^2}{V^2}, \quad (3)$$

where S represents the entropy and c_s the sound speed of the compressed material. We deduce the Mach number,

$$M^2 = \frac{\mathcal{R}}{S} = \left(\frac{D - u}{c_s} \right)^2, \quad (4)$$

and introduce the D’yakov-Kontorovich parameter,

$$h = - \frac{\mathcal{R}}{\mathcal{H}} = j^2 \left. \frac{dV}{dP} \right|_{\mathcal{H}} = -(D - u)^2 \left. \frac{d\rho}{dP} \right|_{\mathcal{H}}. \quad (5)$$

The D’yakov-Kontorovich instability occurs if

$$\frac{1 - (\zeta + 1)M^2}{1 + (\zeta - 1)M^2} = h_c < h < 1 + 2M, \quad (6)$$

where $\zeta = \rho/\rho_0$ denotes the compression of the material. The inequality $h < 1 + 2M$ is always largely satisfied in the cases we consider. The quantity h_c , specified by Kontorovich [18], will be referred to as the “critical parameter” in the following. It is worth mentioning that, according to Landau and Lifshitz [33], the D’yakov-Kontorovich instability is a special form of instability, which is not an instability in the literal sense: the perturbation (ripples) created on the surface, continues indefinitely to emit waves without being damped or amplified. This is why some authors call the D’yakov-Kontorovich unstable shock fronts “neutrally stable”, as opposed to the absolutely stable shock fronts (e.g., in an ideal gas) in which all initial perturbations rapidly decay with time [34,35].

To our knowledge, the D’yakov-Kontorovich instability has never been observed experimentally. Some numerical models have been performed [21–23,34]; for instance, Konyukhov *et al.* [35] carried out hydrodynamic simulations. In a previous paper Konyukhov *et al.* [36] had presented a numerical analysis of the nonlinear instability of shock waves for solid deuterium and for a model medium described by a properly constructed equation of state. In the work described in Refs. [24,25], the D’yakov-Kontorovich instability is supplanted by a corrugation instability for $h > h_c$ when a piston is included in the theory. This remedies the problem of multivalued solutions to projectile impact problems, as described by Refs. [29–31].

The form of the electronic EOS used by Mond *et al.* [26] does not incorporate the quantum details of electronic states (shell structure) and pressure ionization is accounted for by a Gaussian function. In Ref. [37], Das *et al.* consider an equation of state model relying on scaled binding energy for the cold contribution, mean-field theory for the ionic part, and a screened hydrogenic model with ℓ -splitting for the contribution of bound electrons. In their modeling, the free electrons are treated within the nonrelativistic semiclassical Thomas-Fermi model.

In the present work, we investigate D’yakov-Kontorovich instability with an EOS model relying on a full quantum self-consistent calculation of bound and free states solving Dirac equation through a relativistic quantum average-atom model. Our equation-of-state model is presented in Sec. II. In Sec. III, Hugoniot results are given for carbon (C, $Z = 6$), aluminum (Al, $Z = 13$), silicon (Si, $Z = 14$), and niobium (Nb, $Z = 41$) plasmas, and the shock stability is studied for the four elements in light of D’yakov-Kontorovich instability criterion. We find that the instability arises mostly at the end of the ionization of electronic shells, when the relativistic effects start to be important for the electrons. Our conclusions are compared to the ones of previous investigations (see Ref. [37]). In Sec. IV, we show that the accounting for the contribution of a blackbody radiation to the EOS tends to suppress the instability.

II. DESCRIPTION OF THE EQUATION-OF-STATE MODEL

Throughout the paper, atomic units will be used, except that we keep c instead of $1/\alpha$, where c is the speed of light and $\alpha = e^2/(8\pi\epsilon_0 a_0)$ to avoid confusion with the Dirac matrices $\vec{\alpha}$. In our model, the equation of state is built according to

$$\begin{aligned} P(\rho, T) &= P_c(\rho) + P_{\text{th},i}(\rho, T) + P_{\text{th},e}(\rho, T) \\ E(\rho, T) &= E_c(\rho) + E_{\text{th},i}(\rho, T) + E_{\text{th},e}(\rho, T), \end{aligned} \quad (7)$$

where the quantities E_c and P_c (often referred to as the “cold curve”) are, respectively, the pressure and internal energy at the temperature $T = 0$ K and $P_{\text{th},i}$ and $P_{\text{th},e}$ represent, respectively, the thermal ionic and electronic pressures, and $E_{\text{th},i}$ and $E_{\text{th},e}$ the thermal ionic and electronic internal energies. A thermal quantity Y_{th} is defined as

$$Y_{\text{th}}(T) = Y(T) - Y(T = 0). \quad (8)$$

A. Cold curve and ionic contribution

The so-called cold curve is provided by Thomas-Fermi calculations at $T = 0$ K supplemented by the Barnes correction [38,39]. The ideal-gas approximation can be used for sufficiently high temperatures and densities. For dense and condensed media, however, this model is rather crude and it is important to take into account the interactions between ions, which belong to the so-called nonideality effects. To take into account nonideality corrections to the thermal motion of ions, we followed the work of Nikiforov *et al.* [40,41], who used an approximation based on the calculation of the EOS of a one-component plasma (OCP) by the Monte Carlo method [42–44]. In the OCP model, it is assumed that ions with identical charge move in a homogeneous medium that carries a charge of opposite sign.

TABLE I. Values of parameters a_k and b_k , $k = 1, 4$, involved in Eq. (10).

a_1	a_2	a_3	a_4
-0.895929	0.11340656	-0.90872827	0.11614773
b_1	b_2	b_3	b_4
4.666486	13.675411	1.8905603	1.0277554

The authors carried out molecular-dynamics simulations to calculate the distribution function of ions and their interaction energy and derived interpolation formulas on the basis of these results. The ion contribution can be obtained using the Virial theorem; the ionic pressure and internal energy are given by

$$\begin{aligned} P_i(\rho, T) &= \rho k_B T + \frac{\rho}{3} \Delta E_i(\rho, T) \\ E_i(\rho, T) &= \frac{3}{2} k_B T + \Delta E_i(\rho, T), \end{aligned} \quad (9)$$

where the role of ΔE_i is to account for nonideality effects. In computations of the equation of state, it is convenient to modify the interpolation formulas of Hansen [42] for the interaction energy ΔE_i given by the OCP model to ensure that it can still be applied for arbitrary temperatures and densities. The point is that in the OCP model, at values of the nonideality parameter Γ (which is also named coupling parameter and will be explicitly given later) close to 158, a phase transition occurs. Since the physical accuracy of the OCP model is not beyond dispute, in practical computations, to simplify the calculation of the ion contribution to the EOS, one requires that at large values of the parameter Γ , the ion energy E_i will not exceed the asymptotic value $3k_B T$. We have, if the quantity $\Delta E_i(\rho, T)$ is smaller than $3k_B T/2$,

$$\Delta E_i(\rho, T) = k_B T \left[\Gamma^{3/2} \sum_{k=1}^4 \frac{a_k}{(b_k + \Gamma)^{k/2}} - a_1 \Gamma \right], \quad (10)$$

where the coefficients a_k and b_k , $k = 1, 4$ are given in Table I, and $\Delta E_i(\rho, T) = \Delta E_i(T) = 3k_B T/2$ otherwise.

B. Electronic contribution to the EOS: quantum average-atom model

In the present work, we use a relativistic quantum average-atom model [45] following the work of Liberman [46] (see also Ref. [47]). Such a model is often used to calculate the electronic contribution to the equation of state. It relies on a self-consistent computation of the electronic structure. In a spherically symmetric potential, the one-electron wave functions, solutions of Dirac equation, are of the form

$$\psi_s(\vec{r}) \equiv \psi_{j\ell m}(\vec{r}) = \begin{pmatrix} \frac{1}{r} f(r) \Omega_{j\ell m}(\theta, \phi) \\ -\frac{i}{r} g(r) \Omega_{j\ell' m}(\theta, \phi) \end{pmatrix}, \quad (11)$$

where $\Omega_{j\ell m}$ and $\Omega_{j\ell' m}$ are two spinors. j , ℓ , and m are quantum numbers associated, respectively, to the total angular momentum J , to the orbital angular momentum L and its

projection L_z . We define the quantum number ℓ' by

$$\begin{aligned} \ell' &= \ell + 1 & \text{if } j &= \ell + 1/2 \\ \ell' &= \ell - 1 & \text{if } j &= \ell - 1/2. \end{aligned} \quad (12)$$

The radial functions f and g verify the equations

$$\begin{aligned} \frac{df}{dr} &= -\frac{\kappa}{r} f(r) - \frac{V_{\text{eff}}(r) - c^2 - \epsilon}{c} g(r) \\ \frac{dg}{dr} &= \frac{V_{\text{eff}}(r) + c^2 - \epsilon}{c} f(r) + \frac{\kappa}{r} g(r), \end{aligned} \quad (13)$$

where

$$\begin{aligned} \kappa &= -(\ell + 1) & \text{for } j &= \ell + 1/2, \\ \kappa &= \ell & \text{for } j &= \ell - 1/2. \end{aligned} \quad (14)$$

The effective potential V_{eff} is assumed to be constant outside the cavity ($V_{\text{eff}}(r) = V_\infty$ for $r \geq R$). Therefore, the solutions of Dirac equation are known for $r \geq R$, and the equation has to be solved for $r \leq R$. The inside and outside solutions are matched at $r = R$.

The number of bound electrons reads

$$N_{\text{bound}} = \sum_i X_i F(\epsilon_i, \mu), \quad (15)$$

and the number of free electrons reads

$$N_{\text{free}} = \sum_\kappa \int_0^\infty X_\kappa(\epsilon) F(\epsilon, \mu) d\epsilon, \quad (16)$$

where F denotes the Fermi-Dirac distribution,

$$F(\epsilon, \mu) = \frac{1}{e^{\beta(\epsilon - \mu)} + 1}, \quad (17)$$

μ being the chemical potential and $\beta = 1/(k_B T)$. The factor X_i is

$$X_i = \int_{r \leq R} \psi_i^*(\vec{r}) \psi_i(\vec{r}) d^3r, \quad (18)$$

and one has

$$X_\kappa(\epsilon) = 2|\kappa| \int_0^R [P_\kappa^2(\epsilon, r) + Q_\kappa^2(\epsilon, r)] r^2 dr, \quad (19)$$

where

$$\epsilon = c^2 \sqrt{1 + \frac{k^2}{c^2}} \quad \text{or} \quad k = \sqrt{2\epsilon \left(1 + \frac{\epsilon}{2c^2}\right)}, \quad (20)$$

and P_κ and Q_κ represent the radial components of the free-electron spinor.

The chemical potential is obtained from the electroneutrality condition,

$$N_{\text{bound}} + N_{\text{free}} = Z, \quad (21)$$

Z being the atomic number of the considered element. In the usual regime (typically $\mu/(k_B T) = \beta\mu$ less than 250), the Fermi distribution is far from the step function. In that case, Eq. (16) can be split into two parts:

$$N_{\text{free},0} = \sum_\kappa \int_0^{\epsilon_m} X_\kappa(\epsilon) f(\epsilon, \mu) d\epsilon \quad (22)$$

and

$$N_{\text{free},1} = \sum_{\kappa} \int_{\epsilon_m}^{\infty} X_{\kappa}(\epsilon) e^{-\beta(\epsilon-\mu)} d\epsilon, \quad (23)$$

with $\epsilon_m = \max(0, \mu + 10/\beta)$. In Eq. (23), we can assume that $X_{\kappa}(\epsilon)$ can be approximated using the ideal wave functions of an electron gas:

$$P_{\kappa}(\epsilon, r) = k \sqrt{\frac{k}{\pi \epsilon}} j_{\ell}(kr) \quad (24)$$

$$Q_{\kappa}(\epsilon, r) = k \sqrt{\frac{k}{\pi \epsilon}} s_{\kappa} \frac{\epsilon}{kc} j_{\ell'}(kr),$$

where s_{κ} is the sign of κ and we get finally in that case

$$\sum_{\kappa} X_{\kappa} = \frac{1 + \epsilon/c^2}{\pi^2} k \left(\frac{4}{3} \pi R^3 \right), \quad (25)$$

with the maximal orbital quantum number $\ell_m \approx k_m R$, k_m being related to ϵ_m through the second identity of Eq. (20).

The model imposes $f = g = 0$ at $r = 0$ and $r \rightarrow \infty$. Outside the cavity, the radial functions f and g satisfying those boundary conditions are, for bound states, modified Bessel functions of the third kind [66], exponentially decreasing, and, for free states, combinations of Bessel functions of the first and second kinds, with decreasing amplitudes as $r \rightarrow \infty$.

(1) Outside the cavity we have, for $\epsilon < V_{\infty}$ (bound states):

$$f(r) = a_0 c \frac{k}{V_{\infty} - \epsilon} r K_{\ell+1/2}(kr) \quad (26)$$

$$g(r) = a_0 r K_{\ell'+1/2}(kr),$$

where $K_{n+1/2}$ (n being an integer) are modified Bessel functions of the third kind and a_0 the normalization constant

$$a_0 = \frac{1}{\int_0^{\infty} [f^2(r) + g^2(r)]^2 dr}. \quad (27)$$

(2) Outside the cavity we have, for $\epsilon > V_{\infty}$ (free states):

$$f(r) = b_0 c \frac{k}{\epsilon - V_{\infty}} r [\cos(\delta_{\ell}) j_{\ell}(kr) - \sin(\delta_{\ell}) n_{\ell}(kr)] \quad (28)$$

$$g(r) = b_0 r [\cos(\delta_{\ell'}) j_{\ell'}(kr) - \sin(\delta_{\ell'}) n_{\ell'}(kr)],$$

where the normalization factor b_0 and the wave number k are

$$b_0 = \sqrt{\frac{2}{\pi}} \frac{k}{\sqrt{1 + \frac{c^2 k^2}{(\epsilon - V_{\infty})^2}}}$$

$$k = \sqrt{2(V_{\infty} - \epsilon) \left(1 - \frac{(V_{\infty} - \epsilon)}{2c^2} \right)}.$$

The matching of the solutions at the cavity radius provides the spectrum of bound energies and the phase shifts δ_{ℓ} .

The electronic structure (bound and free states) being known, the thermodynamic quantities can be calculated. We compute the internal energy as

$$E = K + U_{c,1} + U_{c,2} + E_{\text{xc}}^{\text{int}}, \quad (29)$$

where the kinetic energy K reads

$$K = \sum_b n_b (\epsilon_b - V_{\infty}) X_b$$

$$+ \sum_{\kappa} \int_0^{\infty} n(\epsilon) (\epsilon - V_{\infty}) X_{\kappa}(\epsilon) d\epsilon$$

$$- \int_{r \leq R} \rho(r) (V_{\text{eff}}(r) - V_{\infty}) d^3 r, \quad (30)$$

with

$$\rho(r) = \sum_{i=b,k} n_i \psi_i(r)^* \psi_i(r), \quad (31)$$

and n_i is the Fermi-Dirac occupation of state i [see Eq. (17)]. We have, more precisely,

$$n_b = \frac{1}{e^{\beta(\epsilon_b - \mu)} + 1} \quad \text{and} \quad n(\epsilon) = \frac{1}{e^{\beta(\epsilon - \mu)} + 1}. \quad (32)$$

The effective potential is given by

$$V_{\text{eff}}(r) = V_c(r) + V_{\text{xc}}(r) - v \quad \text{if } r \leq R,$$

$$V_{\text{eff}}(r) = V_{\infty} \quad \text{if } r > R, \quad (33)$$

with

$$V_c(r) = -\frac{Z}{r} + \int_{r' \leq R} \frac{\rho(r')}{|\vec{r} - \vec{r}'|} d^3 r', \quad (34)$$

$$V_{\text{xc}}(r) = \mu_{\text{xc}}[\rho(r), T], \quad (35)$$

and

$$V_{\infty} = \mu_{\text{xc}}[\bar{\rho}, T], \quad (36)$$

where $\bar{\rho}$ is the density of the jellium. The exchange-correlation chemical potential is

$$\mu_{\text{xc}}[n, T] = \left. \frac{\partial}{\partial n} (n f_{\text{xc}}[n, T]) \right|_T, \quad (37)$$

where f_{xc} is the exchange-correlation free-energy density.

Although the past decades have seen the emergence of increasingly sophisticated formulations for the exchange-correlation effects in the homogeneous electron gas, one finds very few finite-temperature exchange-correlation potentials in the literature (see, for instance, Refs. [48–53]).

Some of the best functionals follow the production of accurate quantum Monte Carlo data, including many-body effects well beyond the so-called “ring” contribution of the earlier based random phase approximation (RPA) works (see, for instance, Ref. [48]). Among them, Ichimaru *et al.* derived formulas [51] based on restricted path integral Monte Carlo (RPIMC) data, which encountered some success in density functional theory. Recently, Karasiev *et al.* proposed a new expression [53] obtained in the same spirit. Their formulas reproduce efficiently the most recent Monte Carlo data (available at the date of their work), with a global error of 0.5%, and a maximum one of 3.3%. Although we did not notice significant differences with Ichimaru’s values, we preferred it for its practical use. Indeed, RPIMC provide discrete values of the internal energy data that were fitted using Padé approximants. The resulting expression was then integrated in $r_s = [3/(4\pi n)]^{1/3}$ to obtain a formula for f_{xc} ,

which presents a rather complicated dependence to the density n of the electron gas, leading to a delicate derivation of the exchange-correlation potential V_{xc} . Karasiev *et al.* used both the internal energy and the kinetic energy RPIMC data to build a set of f_{xc} values on the same grid. The discrete f_{xc} were then fitted using the same Padé approximants as Ichimaru *et al.* The resulting expression is easy to compute and simplifies the derivation of V_{xc} . Both Ichimaru's and Karasiev's formulas respect the correct behavior at $T = 0$ (where the Kohn-Sham exchange contributions are recovered) and at very high T (where V_{xc} and f_{xc} decay as $1/\sqrt{T}$ corresponding to the classical Debye-Hückel limit). Our exchange-correlation functional is nonrelativistic. Indeed, since the relativistic effects are a correction to the exchange correlation their impact is expected to be very small as well. This is the reason why we believe that the nonrelativistic exchange-correlation approximation is sufficient. Although we did not find any exchange-correlation functional including simultaneously finite-temperature and relativistic effects, relativistic effects have been studied in great detail at zero temperature; see, for instance, Ref. [54]. Finally, the parameter ν in Eq. (33) is

$$\nu = f_{xc}[\rho(R), T] - \mu_{xc}[\bar{\rho}, T] + \frac{\bar{\rho}}{\rho(R)}(\mu_{xc}[\bar{\rho}, T] - f_{xc}[\bar{\rho}, T]). \quad (38)$$

The quantity $U_{c,1}$ represents the electron-nucleus Coulomb interaction energy,

$$U_{c,1} = -Z \int_{r \leq R} \frac{\rho(r)}{r} d^3r, \quad (39)$$

and $U_{c,2}$ represents the electron-electron Coulomb interaction energy,

$$U_{c,2} = \frac{1}{2} \iint_{r, r' \leq R} \frac{\rho(r)\rho(r')}{|\vec{r} - \vec{r}'|} d^3r d^3r'. \quad (40)$$

E_{xc}^{int} represents the exchange-correlation energy,

$$E_{xc}^{\text{int}} = \int_{r \leq R} \rho(r) \epsilon_{xc}[\rho(r), T] d^3r, \quad (41)$$

with

$$\epsilon_{xc}[n, T] = \left. \frac{\partial}{\partial \beta} (\beta f_{xc}[n, T]) \right|_n. \quad (42)$$

The total entropy reads

$$S = \sum_b X_b [n_b \ln n_b + (1 - n_b) \ln(1 - n_b)] + \sum_{\kappa} \int_0^{\infty} X_{\kappa}(\epsilon) \{n(\epsilon) \ln n(\epsilon) + [1 - n(\epsilon)] \ln[1 - n(\epsilon)]\} d\epsilon + S_{xc}, \quad (43)$$

S_{xc} being the exchange-correlation entropy,

$$S_{xc} = \int_{r \leq R} \rho(r) s_{xc}[\rho(r), T] d^3r, \quad (44)$$

with

$$s_{xc}[n, T] = - \left. \frac{\partial}{\partial T} f_{xc}[n, T] \right|_n. \quad (45)$$

Both ϵ_{xc} and s_{xc} are easily derived from Karasiev's formula for f_{xc} .

C. Stress-tensor formula for the pressure

To calculate the pressure due to bound and free electrons, we propose here to apply the stress-tensor formula in the relativistic formulation. Blenski and Ishikawa derived a formula in the semirelativistic Pauli approximation [55]. More recently, Maranganti and Sharma have published an elegant way to build the tensor, still in the non-relativistic case [56]. We propose to generalize their approach step by step to apply it to the Dirac equation. Following Ref. [56], let us introduce the density operator $\hat{A}(\vec{r})$ by

$$\begin{aligned} \hat{A}(\vec{r}) &= \frac{1}{2} \{ \hat{A}, \delta(\vec{R} - \vec{r}) \} \\ &= \frac{1}{2} (\hat{A} \delta(\vec{R} - \vec{r}) + \delta(\vec{R} - \vec{r}) \hat{A}), \end{aligned} \quad (46)$$

which satisfies

$$\frac{\partial \hat{A}(\vec{r})}{\partial t} = \frac{1}{i} [\hat{A}(\vec{r}), \hat{H}], \quad (47)$$

\hat{H} being the Hamiltonian of the system. After development of the commutator and anticommutator, we get

$$\frac{\partial \hat{A}(\vec{r})}{\partial t} = \frac{i}{2} \{ \hat{A}, [\hat{H}, \delta(\vec{R} - \vec{r})] \} + \{ [\hat{H}, \hat{A}], \delta(\vec{R} - \vec{r}) \}, \quad (48)$$

and, if \hat{A} and \hat{H} commute,

$$\frac{\partial \hat{A}(\vec{r})}{\partial t} = \frac{i}{2} \{ \hat{A}, [\hat{H}, \delta(\vec{R} - \vec{r})] \}. \quad (49)$$

At this stage, Maranganti and Sharma pursue with the Hamilton operator \hat{H} . We follow the same procedure for the Dirac operator; the commutator $[\hat{H}, \delta]$ is replaced by

$$[c\vec{\alpha} \cdot \vec{p}, \delta(\vec{R} - \vec{r})] = \left[c \sum_{j=1}^3 \alpha_j p_j, \delta(\vec{R} - \vec{r}) \right] \quad (50)$$

or

$$\left[c \sum_{j=1}^3 \alpha_j \left(\frac{\hbar}{i} \nabla_j \right), \delta(\vec{R} - \vec{r}) \right]. \quad (51)$$

In the two latter equations, $\vec{\alpha}$ represents the Dirac matrices

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}, \quad (52)$$

where $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (53)$$

After expanding the right-hand side of Eq. (51), we finally arrive at a conservation relation,

$$\frac{\partial \hat{A}(\vec{r})}{\partial t} + \vec{\nabla} \cdot \hat{T}(\vec{r}) = 0, \quad (54)$$

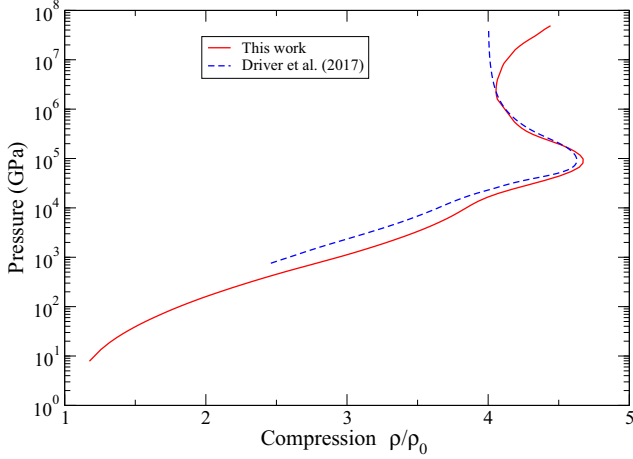


FIG. 1. Pressure along the principal Hugoniot of carbon. Comparison between our results (relativistic quantum average-atom model) and the Hugoniot obtained from density functional theory-molecular dynamics (for $T < 10^6$ K) simulations and path integral monte carlo (for $T > 10^6$ K) by Driver *et al.* [58].

where $\hat{T}(\vec{r})$ represents a tensorial operator whose elements read

$$\hat{T}_{ij} = \frac{c}{2} \{ \hat{A}_i, [\alpha_j, \delta(\vec{R} - \vec{r})] \}. \quad (55)$$

The development relies on the sum of operators of the kind $\hat{G}\delta\hat{D}$ such that

$$\langle \psi | \hat{G}\delta\hat{D} | \phi \rangle = [\hat{G}^+ \psi^*(\vec{R})][\hat{D}\phi(\vec{R})]. \quad (56)$$

The commutator of Eq. (51) becomes an anticommutator since $\hat{p}_j^* = -\hat{p}_j$. The elements \hat{P}_{ij} of the pressure tensor are obtained by replacing the operator \hat{A} by the operator $\hat{p} = \frac{\hbar}{i} \vec{\nabla}$ in Eq. (55); we get

$$\hat{P}_{ij} = \frac{c}{2} \left\{ \frac{1}{i} \nabla_i, \{ \alpha_j, \delta(\vec{R} - \vec{r}) \} \right\}. \quad (57)$$

Finally, the elements \mathcal{P}_{ij} of the pressure tensor read

$$\mathcal{P}_{ij} = \sum_s \langle \psi_s | \hat{P}_{ij} | \psi_s \rangle, \quad (58)$$

where ψ_s are the quadrivectors solutions of Dirac's equation. In the framework of the atom immersed in a spherical cavity, the pressure is given by the only element \mathcal{P}_{rr} of the tensor, evaluated at the radius R of the cavity [57]. After expanding the right-hand side of Eq. (57), we find

$$\begin{aligned} \mathcal{P}_{rr} = \frac{c}{2i} \sum_s \left[- \left(\alpha_r \frac{\partial}{\partial r} \psi_s^* \right) \psi_s - \left(\frac{\partial \psi_s^*}{\partial r} \right) \alpha_r \psi_s \right. \\ \left. + \left(\alpha_r \psi_s^* \right) \left(\frac{\partial \psi_s}{\partial r} \right) + \psi_s^* \left(\alpha_r \frac{\partial}{\partial r} \psi_s \right) \right]_R. \end{aligned} \quad (59)$$

Using the equality

$$\sum_m \Omega_{j\ell m}^*(\theta, \phi) \Omega_{j\ell m}(\theta, \phi) = \frac{2\ell + 1}{4\pi} \delta_{\ell\ell'} \quad (60)$$

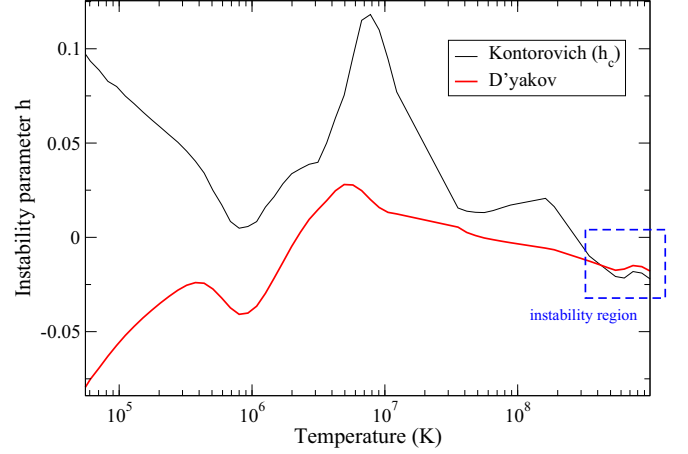


FIG. 2. Value of D'yakov's instability parameter h [17] along the principal Hugoniot of carbon, compared to the critical value h_c as a function of temperature T .

and, following Eq. (11),

$$\alpha_r \psi_{j\ell m} = \begin{bmatrix} -\frac{1}{r} f(r) \Omega_{j\ell m}(\theta, \phi) \\ \frac{i}{r} g(r) \Omega_{j\ell m}(\theta, \phi) \end{bmatrix}, \quad (61)$$

the quantity \mathcal{P}_{rr} can be put in a simple form, depending only on the radial components f and g and their derivatives, evaluated at the radius R of the cavity:

$$\mathcal{P}_{rr} = -c \sum_j \frac{2j+1}{4\pi R^2} \left(f \frac{dg}{dr} - g \frac{df}{dr} \right)_R. \quad (62)$$

A similar expression holds for the free states (with an integral over the free-electron energies). We show in Appendix A how the formula tends, in the nonrelativistic limit, to the form provided by More [57]. Finally, after adding the contribution from exchange-correlation, v and V_∞ , we get, for the total

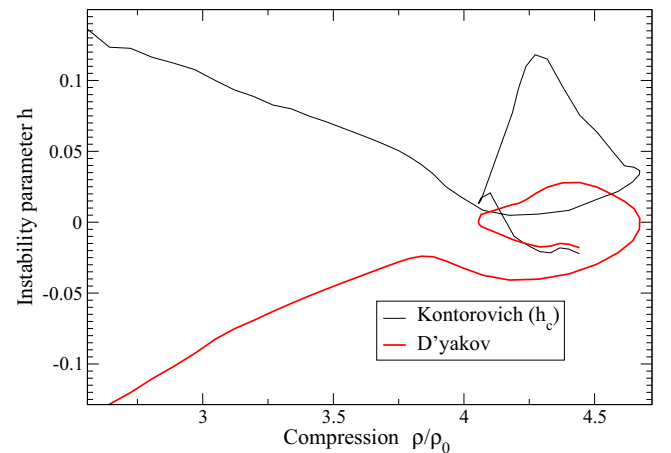


FIG. 3. Value of D'yakov's instability parameter h [17] along the principal Hugoniot of carbon, compared to the critical value h_c as a function of compression ρ/ρ_0 .

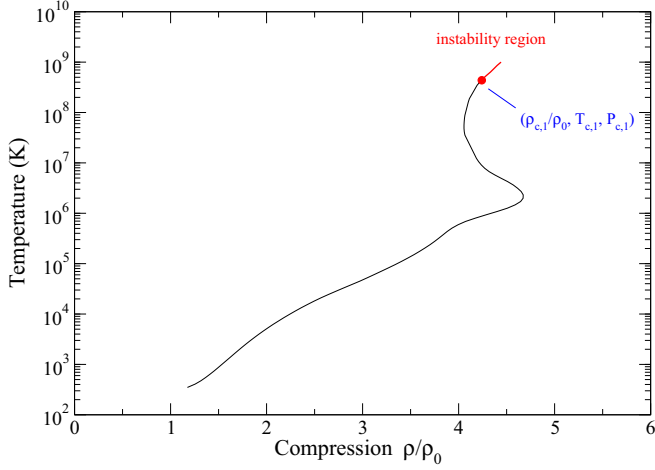


FIG. 4. Temperature and compression along the principal Hugoniot of carbon. The instability region ($h > h_c$) is indicated in red.

electron pressure,

$$P_e = -c \sum_b n_b \frac{2j+1}{4\pi R^2} \left(f \frac{dg}{dr} - g \frac{df}{dr} \right)_R - c \sum_f \int_0^\infty n(\epsilon) \frac{2j+1}{4\pi R^2} \left(f \frac{dg}{dr} - g \frac{df}{dr} \right)_R d\epsilon - \rho(R) f_{xc}[\rho(R), T] - \nu \rho(R) - V_\infty \rho(R), \quad (63)$$

where n_b and $n(\epsilon)$ are provided in Eq. (32). The contributions from exchange and the quantities V_∞ and ν equal the exchange-correlation pressure in the jellium of density $\bar{\rho}$:

$$P_{xc} = -\bar{\rho}(f_{xc}[\bar{\rho}, T] - \mu_{xc}[\bar{\rho}, T]). \quad (64)$$

III. STABILITY OF SHOCK FRONT IN CARBON, ALUMINUM, SILICON, AND NIOBIUM

The Rankine-Hugoniot relation for a planar shock reads

$$E - E_0 = \frac{1}{2}(P + P_0) \left(\frac{1}{\rho_0} - \frac{1}{\rho} \right), \quad (65)$$

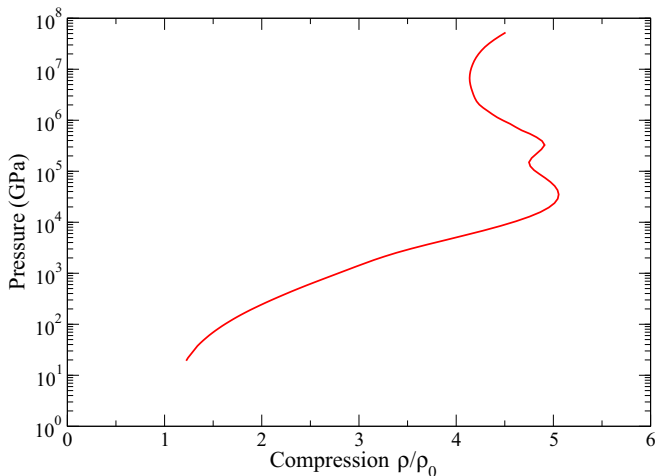


FIG. 5. Principal Hugoniot of aluminum.

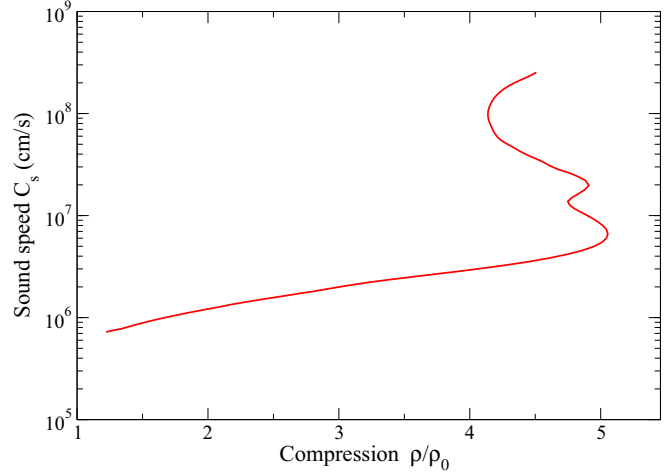


FIG. 6. Sound speed along the principal Hugoniot of aluminum.

where ρ , P , and E represent, respectively, the density, pressure, and internal energy of the shocked material while ρ_0 , P_0 , and E_0 are, respectively, the density, pressure, and internal energy of the pole. The shock and material velocities D and u can be expressed as

$$D = \sqrt{\frac{\rho(P - P_0)}{\rho_0(\rho - \rho_0)}} \quad (66)$$

and

$$u = \frac{P - P_0}{\rho_0 D}. \quad (67)$$

A. Case of carbon

The initial density of carbon in the normal temperature and pressure conditions is chosen to be $\rho_0 = 2.267 \text{ g/cm}^3$. Figure 1 shows the principal Hugoniot curve in the $(\rho/\rho_0, P)$ representation. The figure also displays, for comparison, the Hugoniot obtained from density functional theory-molecular dynamics (DFT-MD) (for $T < 10^6 \text{ K}$) and path integral Monte Carlo (for $T > 10^6 \text{ K}$) by Driver *et al.* [58]. The two shock

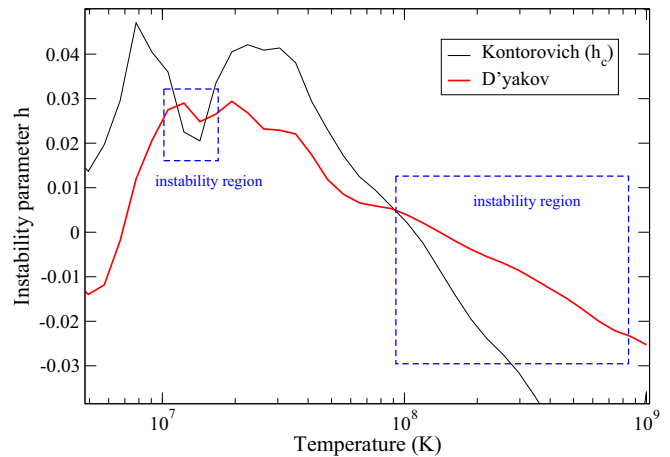


FIG. 7. Value of D'yakov's instability parameter h [17] along the principal Hugoniot of aluminum, compared to the critical value h_c as a function of temperature T .

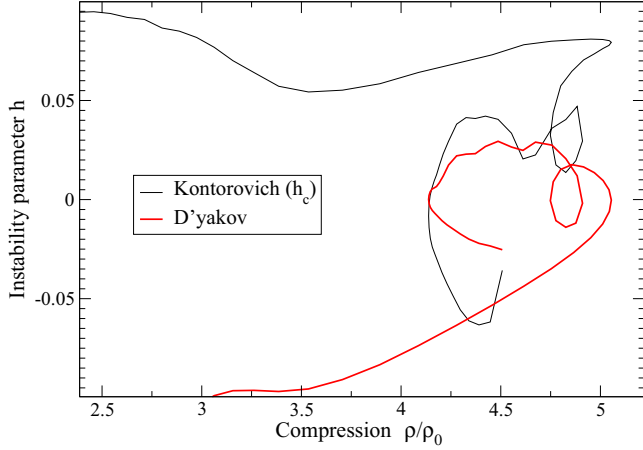


FIG. 8. Value of D'yakov's instability parameter h [17] along the principal Hugoniot of aluminum, compared to the critical value h_c as a function of compression ρ/ρ_0 .

adiabats are very close, also there is a small difference in the maximum compression, which is larger with our approach (by about 1%) in the region of ionization of the L ($n = 1$) shell. At high temperature, the DFT-MD/PIMC Hugoniot does not depart from the asymptote $\rho/\rho_0 = 4$ for tending to the asymptote $\rho/\rho_0 = 7$ because the simulations published in Ref. [58] are nonrelativistic. Figure 2 displays the value of D'yakov's instability parameter [17] along the principal Hugoniot of carbon, compared to the critical value h_c as a function of temperature T . The same two latter quantities are plotted versus compression ρ/ρ_0 in Fig. 3. The correspondence between temperature and density along the principal Hugoniot path is provided by Fig. 4.

We can see that the instability occurs for temperatures above $T_{c,1} = 4.68 \times 10^8$ K, which corresponds to compression $\rho_{c,1}/\rho_0 = 4.37$ and pressure $P_{c,1} = 2.19 \times 10^7$ GPa. The latter compression is slightly greater than the $\rho/\rho_0 = 4$ asymptotic limit of the Hugoniot curve in the nonrelativistic approximation (see Appendix B). In the relativistic case (Dirac equation for the electrons), the asymptote corresponds to

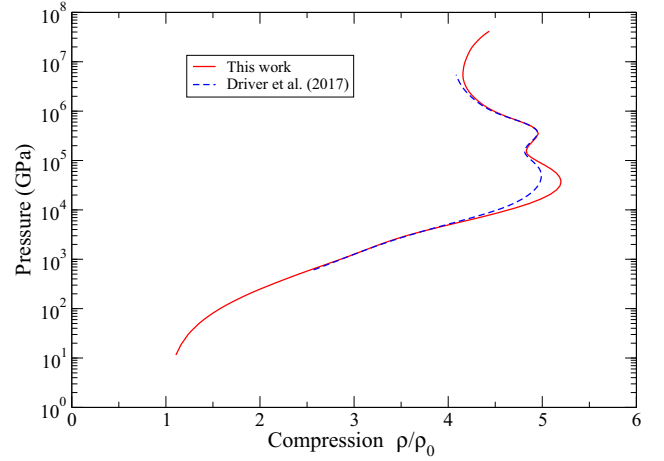


FIG. 10. Principal Hugoniot of silicon. Comparison between our results (relativistic quantum average-atom model) and the Hugoniot obtained from density functional theory-molecular dynamics (for $T < 10^6$ K) simulations and path integral Monte Carlo (for $T > 10^6$ K) by Driver *et al.* [58].

compression 7 (see Appendix B), and compressions much larger than 4 are then possible at high temperatures. This is the reason why, in our previous work [20], we have not detected any instability, since the average-atom model we used relied on Schrödinger equation. The instability occurs at very high temperatures when the principal Hugoniot curve starts to depart from the nonrelativistic asymptote $\rho/\rho_0 = 4$ to reach the asymptote $\rho/\rho_0 = 7$. Typically, the coupling parameter,

$$\Gamma = \frac{Z^{*2} e^2}{r_{ws} k_B T}, \quad (68)$$

is around 0.05 and one can consider that the relativistic effects start to play an important role for $k_B T \geq 0.01 \times c^2 \approx 5$ keV. In the instability region, the ions are almost fully stripped and the most important contribution to the EOS is the electronic part.

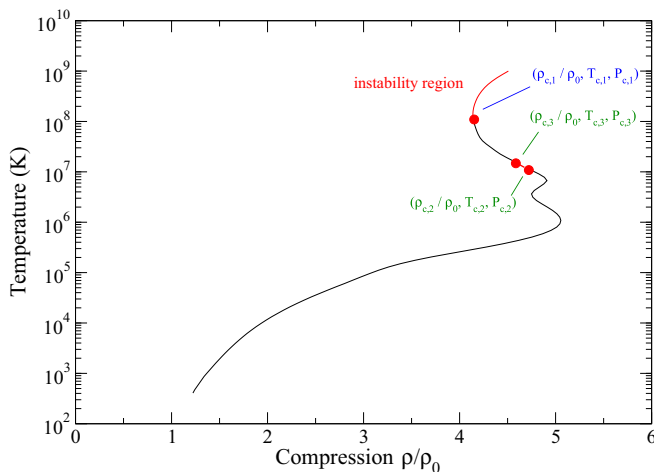


FIG. 9. Temperature and compression along the principal Hugoniot of aluminum. The instability region ($h > h_c$) is indicated in red.

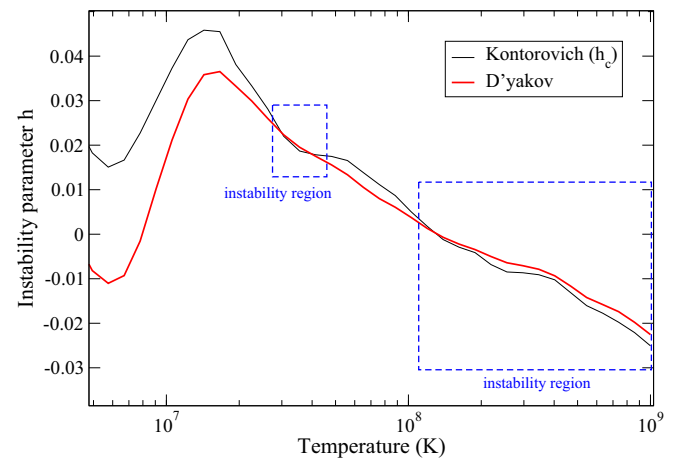


FIG. 11. Value of D'yakov's instability parameter h [17] along the principal Hugoniot of silicon, compared to the critical value h_c as a function of temperature T .

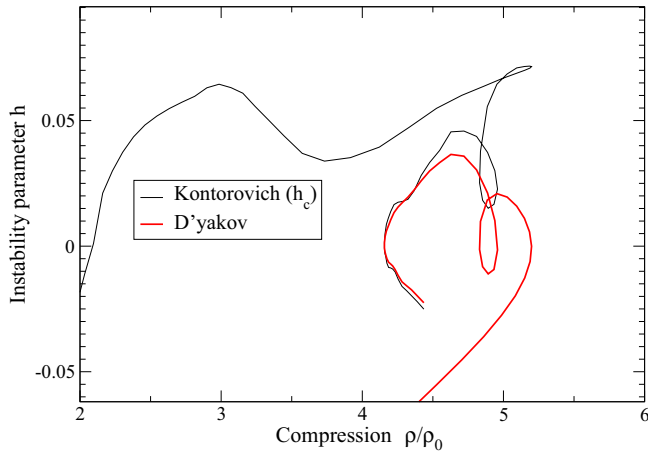


FIG. 12. Value of D'yakov's instability parameter h [17] along the principal Hugoniot of silicon, compared to the critical value h_c as a function of compression ρ/ρ_0 .

B. Case of aluminum

The initial density of aluminum in the normal temperature and pressure conditions is chosen to be $\rho_0 = 2.7 \text{ g/cm}^3$. Figures 5 and 9 show the principal Hugoniot curve, respectively, in the $(\rho/\rho_0, P)$ and $(\rho/\rho_0, T)$ representations. The "shoulders" at high compression are due to the successive ionization of the K ($n = 1$) and L ($n = 2$) shells [59]. As can be seen in Fig. 6, such bumps are also visible in the $(\rho/\rho_0, c_s)$ representation, c_s being the sound speed.

Figure 7 reveals that the instability ($h > h_c$) occurs for temperatures above $T_{c,1} = 1.03 \times 10^8 \text{ K}$, corresponding to $(\rho_{c,1}/\rho_0, P_{c,1}) = (4.14, 4.96 \times 10^6 \text{ GPa})$. In such conditions, the relativistic effects start to play an important role, beyond the cusp point where the bifurcation towards compression 7 starts. This is confirmed by Fig. 8, where the D'yakov's parameter is plotted against compression. Typically, the coupling parameter in this instability region is around 0.3.

We also notice that the instability occurs as well for temperatures between $T_{c,2} = 1.22 \times 10^7 \text{ K}$ and $T_{c,3} = 1.43 \times 10^7 \text{ K}$,

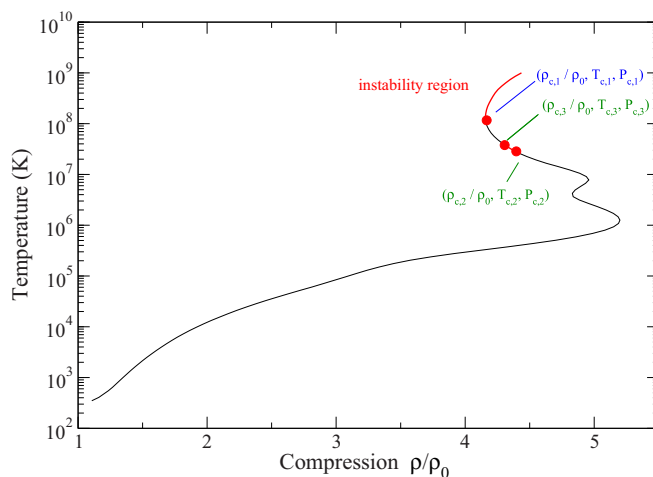


FIG. 13. Temperature and compression along the principal Hugoniot of silicon. The instability region ($h > h_c$) is indicated in red.

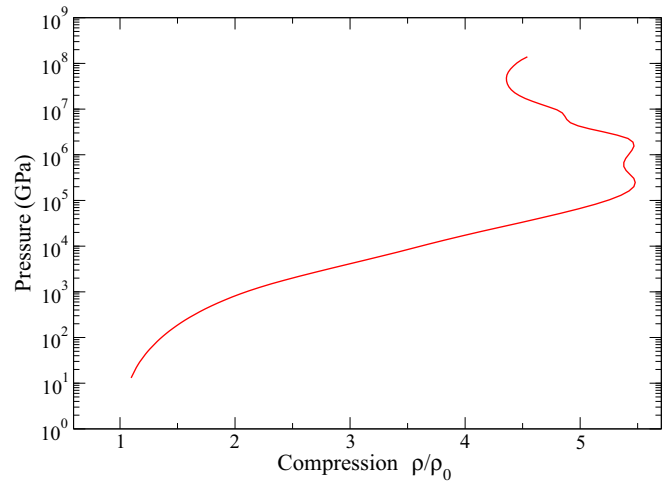


FIG. 14. Principal Hugoniot of niobium.

corresponding to $(\rho_{c,2}/\rho_0, P_{c,2}) = (4.67, 6.33 \times 10^5 \text{ GPa})$ and $(\rho_{c,3}/\rho_0, P_{c,3}) = (4.61, 7.35 \times 10^5 \text{ GPa})$, respectively (the matching between temperature and density along the principal Hugoniot path is provided by Fig. 9).

In the interesting study carried out by Das *et al.* [37], the authors find, for aluminum, two instability regions: the first one exists for a much lower temperature than we find (around $T \approx 150 \text{ eV}$, i.e., about $1.7 \times 10^6 \text{ K}$), after which D'yakov's parameter falls below the critical value h_c , and a second instability region starts around $T \approx 550 \text{ eV}$, i.e., $6.4 \times 10^6 \text{ K}$. Since this occurs in the conditions where ionization of K and L shells is important, we agree with the statement that D'yakov's instability is strongly connected to quantum electronic properties, but we find that the shock becomes unstable for much higher temperatures. This is probably due to the differences between our models (screened hydrogenic versus quantum bound states and nonrelativistic versus relativistic).

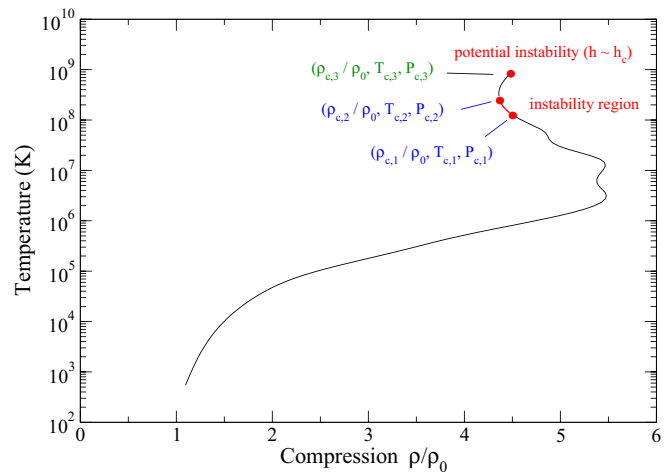


FIG. 15. Value of D'yakov's instability parameter h [17] along the principal Hugoniot of niobium, compared to the critical value h_c as a function of compression ρ/ρ_0 .

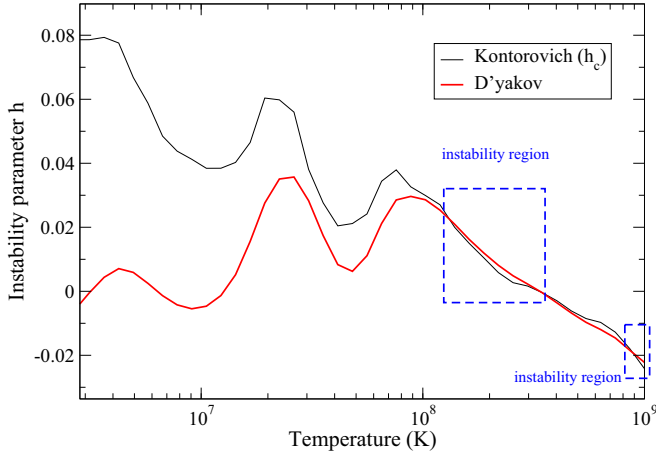


FIG. 16. Value of D'yakov's instability parameter h [17] along the principal Hugoniot of niobium, compared to the critical value h_c as a function of temperature T .

C. Case of silicon

The initial density of silicon in the normal temperature and pressure conditions is chosen to be $\rho_0 = 2.33 \text{ g/cm}^3$. Figure 10 displays our Hugoniot curve and the one obtained from PIMC / DFT-MD computations by Driver *et al.* As for carbon, our approach predicts a higher maximal compression (about 4%).

Figure 11 indicates that the instability ($h > h_c$) occurs for temperatures above $T_{c,1} = 1.39 \times 10^8 \text{ K}$, corresponding to $(\rho_{c,1}/\rho_0, P_{c,1}) = (4.16, 5.93 \times 10^6 \text{ GPa})$, after the departure from compression 4 to compression 7. The D'yakov's parameter is plotted against compression in Fig. 12 and the temperature range in which the system becomes unstable can be viewed in Fig. 13. This is not surprising since the atomic numbers of aluminium and silicon differ only by one. Typically, the coupling parameter in the instability region is around 0.3.

As for aluminium, we find a narrow region of instability between $T_{c,1} = 2.97 \times 10^7 \text{ K}$ and $T_{c,2} = 4 \times 10^7 \text{ K}$, corresponding to $(\rho_{c,2}/\rho_0, P_{c,2}) = (4.36, 1.36 \times 10^6 \text{ GPa})$ and $(\rho_{c,3}/\rho_0, P_{c,3}) = (4.29, 1.81 \times 10^6 \text{ GPa})$, respectively (the matching between temperature and density along the principal Hugoniot path is provided by Fig. 13).

D. Case of niobium

The initial density of niobium in the normal temperature and pressure conditions is chosen to be $\rho_0 = 8.57 \text{ g/cm}^3$. Figures 14 and 15 display the principal Hugoniot curve, respectively, in the $(\rho/\rho_0, P)$ and $(\rho/\rho_0, T)$ representations. The D'yakov's instability parameter [17] and the critical value h_c along the principal Hugoniot of niobium are plotted as a function of temperature T in Fig. 16 and versus compression ρ/ρ_0 in Fig. 17.

The instability occurs for temperatures between $T_{c,1} = 1.39 \times 10^8 \text{ K}$ (compression $\rho_{c,1}/\rho_0 = 4.47$ and $P_{c,1} = 1.97 \times 10^7 \text{ GPa}$) and $T_{c,2} = 2.97 \times 10^8 \text{ K}$, for which the compression is $\rho_{c,2}/\rho_0 = 4.36$ and the pressure $P_{c,2} = 4.11 \times 10^7 \text{ GPa}$. As for carbon and silicon, the compression in that range is greater than the nonrelativistic $\rho/\rho_0 = 4$ asymptotic limit of the Hugoniot curve. Here, also, the instability occurs at very high temperatures just before the principal Hugoniot curve

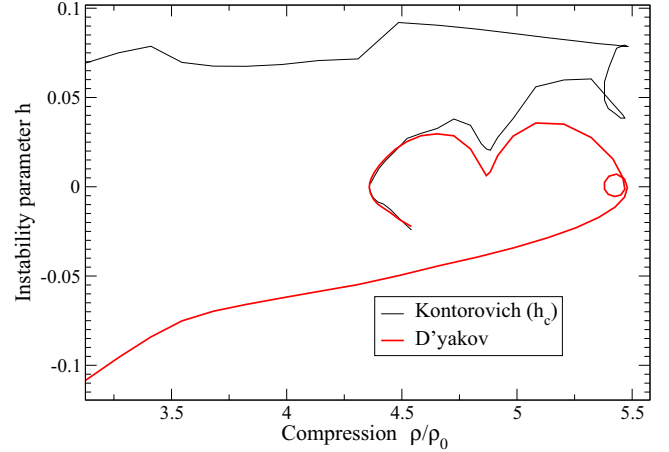


FIG. 17. Value of D'yakov's instability parameter h [17] along the principal Hugoniot of niobium, compared to the critical value h_c as a function of compression ρ/ρ_0 .

starts to depart from the $\rho/\rho_0 = 4$ asymptote to reach the limit $\rho/\rho_0 = 7$. Typically, the coupling parameter in the instability region is around 2–3. In that case the nonideality correction to the ionic EOS [see Eqs. (9) and (10)] are important.

At the end of the Hugoniot curve, i.e., at $T_{c,3} = 10^9 \text{ K}$, where compression is $\rho_{c,3}/\rho_0 = 4.54$ and pressure $P_{c,3} = 1.39 \times 10^8$, we see also the beginning of another instability region.

IV. RADIATIVE PRESSURE AND INTERNAL ENERGY

Most of the earlier work on the subject [22,24,25] was focused on the low-temperature range. Mond *et al.* [26] studied shock waves propagating in room-temperature argon, with post-shock temperatures not exceeding several eV. Konyukhov *et al.* who approximated a realistic EOS for magnesium with a van der Waals model, found the D'yakov-Kontorovich unstable regions at plasma temperatures below 20 eV [35]. At such low temperatures, one can safely neglect the energy density and pressure of the plasma radiation. The shock waves studied here are so strong that the post-shock plasma in thermodynamic equilibrium must be radiation-dominated. However, it is not clear to us whether the plasma radiation should be accounted for or not in the Hugoniot energy balance. For instance, Das *et al.* [37] did not include it in their study of D'yakov-Kontorovich instability. This is justified because their temperatures are lower than $1.1 \text{ keV} \approx 1.28 \times 10^7 \text{ K}$, which corresponds to the end of the signature of the shell structure, before the relativistic effects start to play a role. The impact on the radiation field is important in a radiative-hydrodynamics simulation, and is different at each time step and spatial mesh. Usually, in ICF, its distribution is far from a Planckian. In the diffusion approximation, the one-dimensional radiative transfer equation reads

$$\frac{dI_v}{dx} = -\kappa_v I_v + j_v, \quad (69)$$

I_v being the intensity of the radiation, κ_v its opacity, and j_v its emissivity. The solution of such an equation, for an homogeneous medium and assuming that κ_v and j_v are related

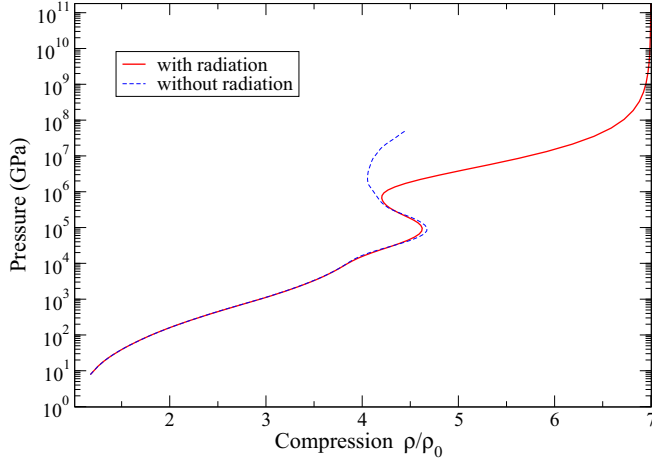


FIG. 18. Principal Hugoniot of carbon with and without blackbody radiation.

by Kirchoff's law,

$$j_v = B_v \kappa_v, \quad (70)$$

where B_v is Planck's distribution function, is given by

$$I_v = B_v [1 - e^{-\rho L \kappa_v}], \quad (71)$$

where ρ is the density of the material and L its thickness. If $\rho L \kappa_v \gg 1$, the plasma is optically thick and one has $I_v = B_v$ and the radiation is the one of a blackbody.

In Sec. III, we have not accounted for the energy and pressure of the equilibrium radiation when calculating the Hugoniot shock adiabats. This means that we have assumed implicitly that the shocked plasma is optically thin to its own radiation. Unlike the optically thick plasma, an optically thin plasma cannot be in a steady state; it is radiatively cooled, losing its thermal energy with time. To justify the steady-state Hugoniot calculations that ignore the cooling, one has to consider a sufficiently small depth of the shocked plasma layer and that the radiation energy loss can be neglected while the plasma flows through it. However, to apply the D'yakov-Kontorovich theory, this depth should be much larger than both the shock width and the transverse perturbation wavelength.

In the case where the plasma is optically thick, it may be relevant to include radiation in the EOS of the material when computing the Hugoniot [60], through a blackbody radiation EOS model, as used for instance by Das and Menon [61]. This should give insight, at least qualitatively, into the impact of radiation on the instability criterion. The electrons in the plasma produce radiation heating via Bremsstrahlung and also reach equilibrium with the plasma via inverse Bremsstrahlung and Compton scattering process. As pointed out by Das and Menon [61], the timescale for the equilibration of radiation with matter is generally of the order of 10^{-13} to 10^{-15} s, which is negligible in comparison to the timescale of shock propagation 10^{-9} to 10^{-6} s and hence justifies that the matter exists in equilibrium with radiation. Under equilibrium condition, the energy density of radiation depends on the temperature of the material. When an intense shock is launched, the temperature becomes so high that the energy density and pressure of radiation become comparable to the internal energy and pressure of electrons, thereby

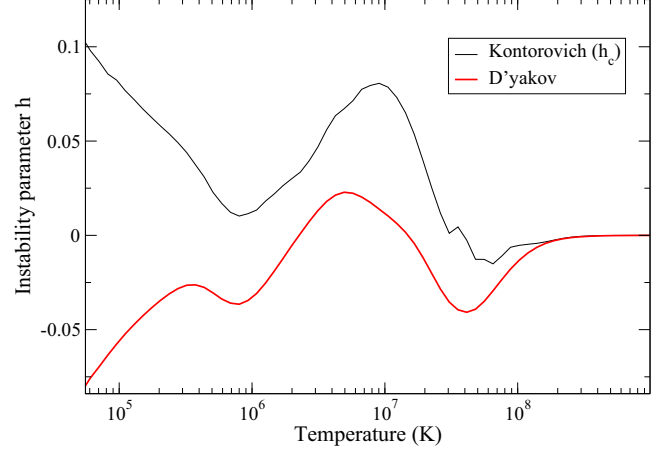


FIG. 19. Value of D'yakov's instability parameter h [17] along the principal Hugoniot of carbon, compared to the critical value h_c as a function of temperature T . The EOS model includes blackbody radiation.

affecting both the EOS and Hugoniot. The derivation of the Hugoniot relations assumes that the post-shock matter is in full thermodynamic equilibrium, that is, it must be optically thick to its own radiation. The local thermodynamic equilibrium of the plasma with the radiation implies a Planckian spectrum corresponding to the post-shock temperature.

The pressure and energy of equilibrium radiation can be obtained using Stefan-Boltzmann law and the energy density of radiation is given by

$$W = \sigma T^4, \quad (72)$$

where $\sigma = \frac{\pi^2 k_B^4}{60 \hbar^3 c^2} = 5.67 \times 10^{-8} \text{ W/m}^2/\text{K}^4$ is Stefan-Boltzmann's constant. The free energy of the photon gas in a volume V at a temperature T is equal to

$$F_{\text{rad}} = \frac{k_B T V}{\pi^2 c^3} \int_0^\infty \omega^2 \ln [1 - e^{-\frac{\hbar \omega}{k_B T}}] d\omega = -P V. \quad (73)$$

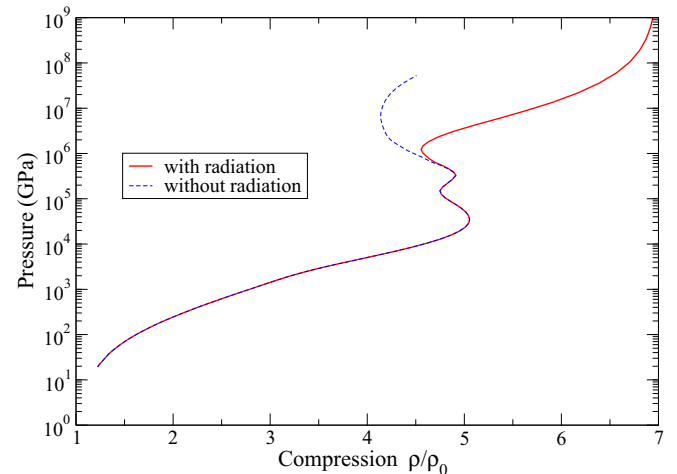


FIG. 20. Principal Hugoniot of aluminum with and without blackbody radiation.

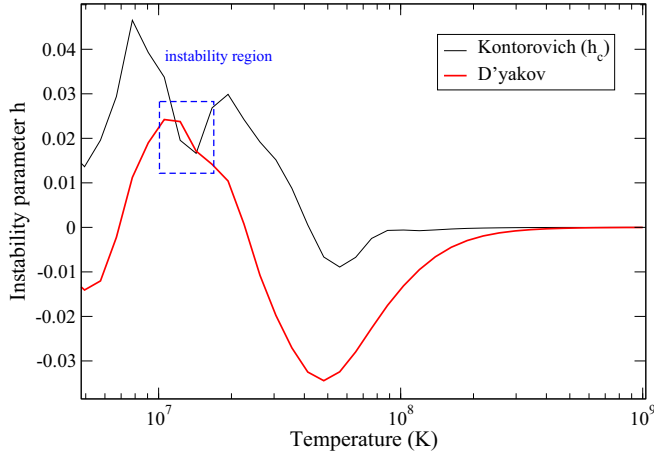


FIG. 21. Value of D'yakov's instability parameter h [17] along the principal Hugoniot of aluminum, compared to the critical value h_c as a function of temperature T . The EOS model includes blackbody radiation.

The entropy reads

$$S_{\text{rad}} = - \left. \frac{\partial F_{\text{rad}}}{\partial T} \right|_V = \frac{16\sigma}{3c} T^3 V, \quad (74)$$

which gives for the internal energy

$$E_{\text{rad}} = F_{\text{rad}} + T S_{\text{rad}} = -3F_{\text{rad}} \quad (75)$$

and for the pressure

$$P_{\text{rad}} = \frac{1}{3V} E_{\text{rad}} = \frac{4\sigma}{3c} T^4. \quad (76)$$

Identifying Eq. (76) with the ideal-gas law, we obtain

$$\frac{P_{\text{rad}} V}{(\gamma - 1)} = E_{\text{rad}}, \quad (77)$$

with $\gamma = 4/3$. The pressure P_{rad} [see Eq. (76)] of the blackbody radiation at the temperature of $T = 43 \text{ keV}$ (about $5 \times 10^8 \text{ K}$) is equal to $1.58 \times 10^{10} \text{ GPa} = 158 \text{ Tbar}$, which is orders of magnitude higher than the ‘‘matter’’ pressure [contribution of

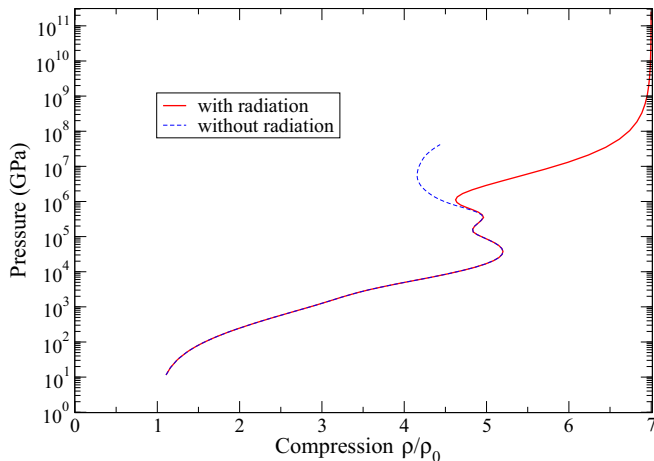


FIG. 22. Principal Hugoniot of niobium with and without blackbody radiation.

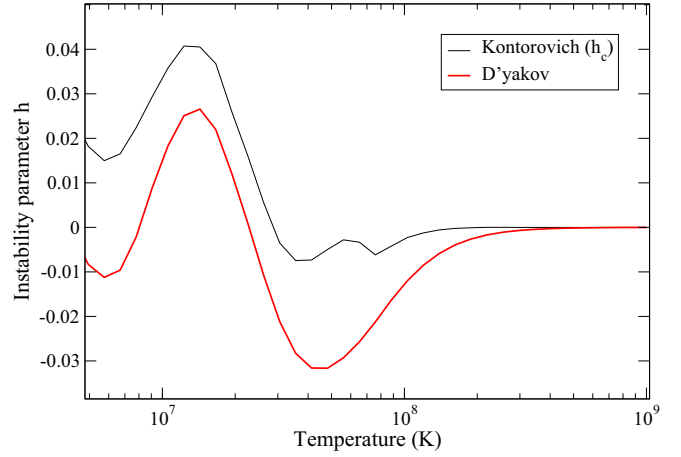


FIG. 23. Value of D'yakov's instability parameter h [17] along the principal Hugoniot of silicon, compared to the critical value h_c as a function of temperature T . The EOS model includes blackbody radiation.

ions and electrons to the pressure, see Eqs. (9) and (63)]. We can see in Figs. 18, 20, 22, and 24 that when the EOS of a photon gas is taken into account, the shock adiabat is strongly affected at high temperature, and the bifurcation to the $\rho/\rho_0 = 7$ asymptote starts at lower temperatures and with a higher slope than in the case where only ions and electrons are taken into account [see Eqs. (1), (5), (10), and (14) of Sec. III].

When radiation is included in the EOS, the instability does not occur anymore at high temperature (see Figs. 19, 21, 23, and 25), which can be proven analytically (see Appendix C). There is a difference between aluminum and silicon; for silicon, the instability disappeared completely (see Fig. 21), but a narrow instability region (around 10^7 K) remains for aluminum (see Fig. 23).

However, it is worth mentioning that the assumption of a large optical thickness, for a plasma of higher-than-solid density, is far from obvious. For instance, in the case of an aluminum plasma at a temperature of $2 \times 10^7 \text{ K}$ and a compression close to 5, the Rosseland mean free path λ_R is

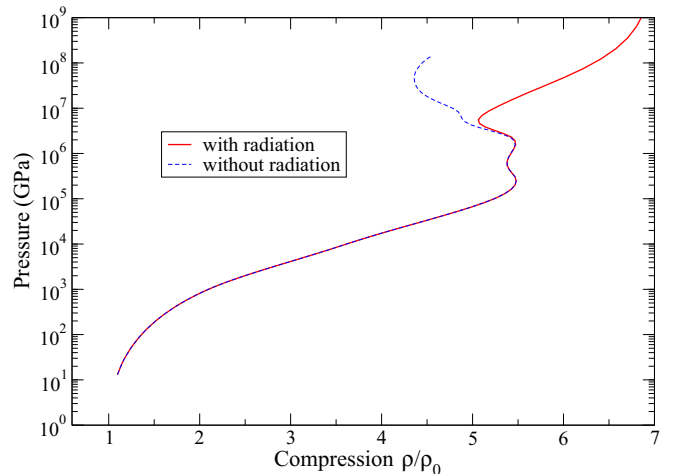


FIG. 24. Principal Hugoniot of niobium with and without blackbody radiation.

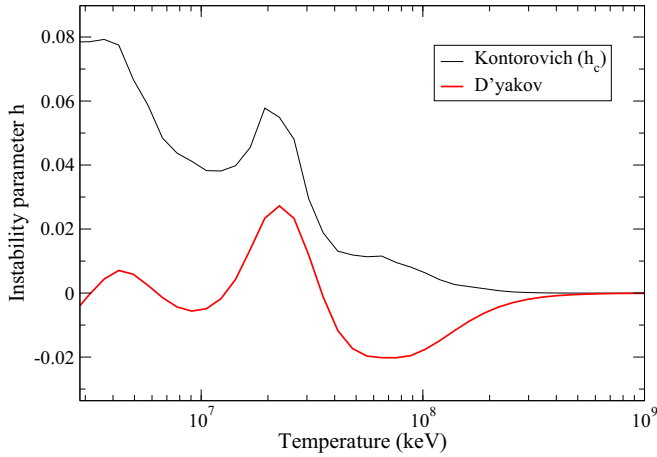


FIG. 25. Value of D'yakov's instability parameter h [17] along the principal Hugoniot of niobium, compared to the critical value h_c as a function of temperature T . The EOS model includes blackbody radiation.

of the order of 0.45 cm. At a pressure near 10 Gbar, when the Hugoniot curves with and without radiation diverge (see Fig. 20), the shock velocity is around 700 km/s. For the upper bound of the shock propagation time $1 \mu\text{s}$, the shock travels $L = 70$ cm and thus $L \gg \lambda_R$, i.e., the plasma is optically thick. However, considering the abovementioned lower bound of the shock propagation time 1 ns, the shock travels 0.07 cm and thus $L \ll \lambda_R$, i.e., the plasma is optically thin. In conditions typical for ICF experiments [3], the laser pulse duration is around 5 ns, and therefore the plasma is neither optically thick nor thin. Only a radiation-hydrodynamics simulation can provide reliable information about the radiation field.

V. CONCLUSION

In this paper, we have studied the conditions for the occurrence of the D'yakov-Kontorovich hydrodynamic instability via acoustic emission in hot and dense plasmas employing an accurate EOS for electrons, based on a full quantum self-consistent relativistic (Dirac) average-atom model. The pressure is determined using the relativistic stress-tensor formula. We agree with the assertion of Das *et al.* [37] that the instability is related to thermal as well as pressure ionization (i.e., that the shock waves become unstable for temperatures and pressures where sudden ionization of electronic shells occurs), but our conclusions are different as concerns the conditions in which the instability occurs. Our model predicts that the shock becomes unstable for higher temperatures, when the Hugoniot curve departs from the nonrelativistic asymptote $\rho/\rho_0 = 4$ toward the limit $\rho/\rho_0 = 7$, i.e., almost beyond the successive ionization of the electronic shells. In other words, we find that a shock becomes unstable only for very high temperatures, at which relativistic effects on the EOS are significant. Absorption of energy from the shock wave due to ionization is a prerequisite for the occurrence of the instability, but the accounting for relativistic effects is of crucial importance. The differences between the present conclusions and the ones from Ref. [37] or from our previous work [20], stem from the fact that in the models used in the two latter

references, the electrons were described in a nonrelativistic approximation: bound electrons were treated *via* the screened hydrogenic model with ℓ splitting in Ref. [37], and *via* Schrödinger equation in Ref. [20], while in both cases free electrons were modeled by the nonrelativistic Thomas-Fermi model. In the present work, both bound and free electrons are described in the framework of relativistic quantum mechanics (Dirac equation in a self-consistent potential). We studied four elements, carbon, aluminum, silicon, and niobium, and found that the instability occurs in a rather narrow range of thermodynamic conditions. Although we cannot draw any definitive conclusion from only four examples, it seems that the instability is more likely to take place at high temperature, which is consistent with the results of Das *et al.* for beryllium and aluminum, but in our case the instability occurs mostly at the end of the ionization of electronic shells, in the range where relativistic effects start to have an impact on pressure and internal energy. In such conditions, if the plasma is optically thick, the contribution of radiation should be accounted for in the energy balance. We have thus studied the impact of a blackbody radiation on the occurrence of the instability and it turns out that the Hugoniot curve departs very brutally from the compression 4 to the compression 7, preventing the instability to occur (except in a very narrow range at lower temperature for aluminum). We conclude that an accurate electronic EOS and radiative opacity is essential for a proper investigation of shock instability. Assuming that the D'yakov-Kontorovich instability exists in plasmas, its study may be a stringent test of theoretical EOS models (especially as concerns the electronic contribution), although the present works are only predictions, due to the fact that experiments in such extreme conditions remain challenging.

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APPENDIX A: NONRELATIVISTIC LIMIT OF THE STRESS-TENSOR FORMULA

Setting $V = V_{\text{eff}}(R)$, $f = f(R)$, and $g = g(R)$, the derivatives $\frac{df}{dr}$ and $\frac{dg}{dr}$ at the radius of the cavity are given by

$$\left. \frac{df}{dr} \right|_R = -\frac{\kappa}{R}f + \frac{\epsilon + c^2 - V}{c}g \quad (\text{A1})$$

$$\left. \frac{dg}{dr} \right|_R = \frac{\kappa}{R}g - \frac{\epsilon - c^2 - V}{c}f.$$

In the nonrelativistic limit: $\epsilon = \frac{k^2}{2}$, $V \ll c^2$, the preceding system becomes

$$\left. \frac{df}{dr} \right|_R = -\frac{\kappa}{R}f + 2cg$$

$$\left. \frac{dg}{dr} \right|_R = \frac{\kappa}{R}g - \frac{1}{c} \left(\frac{k^2}{2} - V \right) f, \quad (\text{A2})$$

and we deduce

$$\left(f \frac{dg}{dr} - g \frac{df}{dr}\right)_R = -\frac{1}{2c} \left[\left(k^2 - \frac{\kappa^2}{R^2}\right) f^2 + \left(\frac{df}{dr}\right)^2 \right] + \frac{V}{c} f^2. \quad (\text{A3})$$

Finally, noticing that

$$\begin{aligned} \sum_j (2j+1) \cdots &= 2 \sum_\ell (2\ell+1) \cdots \\ \sum_j (2j+1) \kappa^2 \cdots &= 2 \sum_\ell (2\ell+1) (\ell^2 + \ell + 1) \cdots, \end{aligned} \quad (\text{A4})$$

we check that, assuming $V_{\text{eff}}(R) = 0$, Eq. (63) tends to the one given by Eq. (65) of More's article [57], i.e., for the free states:

$$P_{NR} = \frac{1}{2} \sum_\ell \frac{2(2\ell+1)}{4\pi R^2} \int_0^\infty n(\epsilon) \times \left\{ \left(\frac{df}{dr}\right)_R^2 + \left[k^2 - \frac{\ell(\ell+1)+1}{R^2} \right] f(R)^2 \right\} d\epsilon. \quad (\text{A5})$$

The nonrelativistic stress-tensor expression of pressure was used in several equation-of-state models (see, for instance, Refs. [62–64]).

APPENDIX B: PROOF OF THE ASYMPTOTIC LIMITS $\rho/\rho_0 = 4$ AND $\rho/\rho_0 = 7$ FOR THE ELECTRON GAS

In this Appendix, we show that, when the radiation is not taken into account in the EOS (i.e., if we consider only ions and electrons), when the relativistic effects are negligible, the shock adiabat in the pressure-density representation tends to the limit $\rho/\rho_0 = 4$ and that the asymptote $\rho/\rho_0 = 7$ can be reached only if the electrons are ultra-relativistic.

At high temperature, $E \gg E_0$, $P \gg P_0$, and the Hugoniot relation Eq. (65) can be written

$$\frac{\rho}{\rho_0} = 1 + \frac{2E\rho}{P}, \quad (\text{B1})$$

and the electronic contribution to the EOS largely dominates the ionic one. Let us consider, first the nonrelativistic limit, and then the relativistic one.

(1) Nonrelativistic limit:

Using the nonrelativistic ideal-gas equation of state:

$$\begin{aligned} P &= \rho k_B T \\ E &= \frac{3}{2} \rho k_B T, \end{aligned} \quad (\text{B2})$$

we get the asymptote

$$\frac{\rho}{\rho_0} = 4. \quad (\text{B3})$$

(2) Relativistic limit:

The equation of state of the relativistic ideal gas is (see, for instance, Ref. [65]):

$$\begin{aligned} P &= \rho k_B T \\ E &= c^2 \left\{ \frac{K_1(u)}{K_2(u)} + \frac{3}{u} - 1 \right\} \quad \text{with} \quad u = \frac{c^2}{k_B T}, \end{aligned} \quad (\text{B4})$$

where $K_n(u)$ is the Bessel function of the third kind

$$K_n(u) = \frac{2^n u^n \Gamma(n+1/2)}{\sqrt{\pi}} \int_0^\infty \frac{\cos \xi}{(\xi^2 + u^2)^{n+1/2}} d\xi, \quad (\text{B5})$$

Γ being the usual Gamma function [66]. The entropy and the specific heat are, respectively,

$$S = N k_B \left\{ \ln \left[\frac{4\pi}{\rho} \left(\frac{mc}{h}\right)^3 \frac{K_2(u)}{u} \right] + 4 + u \frac{K_1(u)}{K_2(u)} \right\} \quad (\text{B6})$$

and

$$C_V = N k_B u \left\{ u + \frac{3}{u} - \frac{K_1(u)}{K_2(u)} \left[3 + u \frac{K_1(u)}{K_2(u)} \right] \right\}. \quad (\text{B7})$$

At very high temperatures ($u \ll 1$), we can use the approximation

$$K_n(u) \approx \Gamma(n) \left(\frac{u}{2}\right)^{-n}, \quad (\text{B8})$$

where $\Gamma(n+1) = n!$. Therefore, we have

$$E \approx c^2 \frac{3}{u} = 3k_B T, \quad (\text{B9})$$

and the asymptote in that case is, using Eq. (B1),

$$\frac{\rho}{\rho_0} = 7. \quad (\text{B10})$$

In the present work, we do not reach conditions in which the electrons are ultra-relativistic. The strong-shock compression limit of 7 is approached when the pressure of the Planckian radiation begins to dominate. The reason is that at the temperatures much less than the rest mass of the electron 0.511 MeV, the plasma particles, rather than the photons, are responsible for the dissipations that form the shock front. However, it does not mean that the shock wave becomes relativistic or that it propagates through a photon gas. It is worth mentioning that the relativistic and nonrelativistic limits of compression ratios of an ideal gas can be presented in a general form as [67]

$$\frac{P}{P_0}(\zeta) = \frac{[6 + R(\lambda)]\zeta - R(\lambda)}{6 + R(\lambda) - \zeta R(\lambda)}, \quad (\text{B11})$$

where $\zeta = \rho/\rho_0$, $\lambda = k_B T/c^2$ and the function $R(\lambda)$ is given in the Appendix of Ref. [67]. We have $R(\lambda) \rightarrow 2$ as $\lambda \rightarrow 0$ and $R(\lambda) \rightarrow 1$ as $\lambda \rightarrow \infty$.

We can also evoke the fact that the strong shock compression limit for an ideal gas EOS is

$$\frac{\gamma + 1}{\gamma - 1}, \quad (\text{B12})$$

where γ is the polytropic exponent. For a monoatomic gas, $\gamma = 5/3$, so the compression limit is 4. For a photon gas in equilibrium, i.e., for blackbody radiation, $\gamma = 4/3$, hence the limiting compression equals 7.

APPENDIX C: PARAMETERS h AND h_c IN THE CASE WHERE RADIATION IS INCLUDED IN THE EOS

The Rankine-Hugoniot relations, assuming $u_0 = 0$, read

$$VD = V_0(D - u) \quad (\text{C1a})$$

$$(P - P_0)V_0 = Du \quad (\text{C1b})$$

$$(P + P_0)(V_0 - V) = 2(E - E_0), \quad (\text{C1c})$$

or equivalently

$$(P + P_0)(V_0 - V) = 2(E - E_0) \quad (\text{C2a})$$

$$VD = V_0(D - u) \quad (\text{C2b})$$

$$u^2 = -(P - P_0)(V - V_0), \quad (\text{C2c})$$

where the EOS of the pole (P_0, E_0) is dominated by ions and electrons, and where the temperature is sufficiently high so that the point (P, E) on the shock adiabat is dominated by the radiation field.

We have, using Eq. (C2b) and (C2c),

$$(D - u)^2 = \frac{(P - P_0)V}{\zeta - 1}, \quad (\text{C3})$$

where $\zeta = V_0/V = \rho/\rho_0$ is the compression. Taking $E = E_{\text{rad}}$ [see Eqs. (77) and (B9)] and differentiating Eq. (C2a) yields

$$dP(V_0 - V) - (P + P_0)dV = 6PdV + 6VdP, \quad (\text{C4})$$

and since

$$\left. \frac{d\rho}{dP} \right|_{\mathcal{H}} = -\frac{1}{V^2} \left. \frac{dV}{dP} \right|_{\mathcal{H}}, \quad (\text{C5})$$

we obtain

$$\left. \frac{d\rho}{dP} \right|_{\mathcal{H}} = \frac{7 - \zeta}{(P_0 + 7P)V}. \quad (\text{C6})$$

The D'yakov instability parameter

$$h = -(D - u)^2 \left. \frac{d\rho}{dP} \right|_{\mathcal{H}}, \quad (\text{C7})$$

is therefore equal to

$$h = \frac{\left(\frac{P}{P_0} - 1\right)(7 - \zeta)}{\left(1 + 7\frac{P}{P_0}\right)(1 - \zeta)}. \quad (\text{C8})$$

Combining Eqs. (77) and (C2a) gives

$$\frac{P}{P_0} = \frac{1 - (1 + 2\chi_0)\zeta}{\zeta - 7}, \quad (\text{C9})$$

where $\chi_0 = \frac{E_0}{P_0 V_0}$ and finally

$$h = \frac{(\zeta - 7)[(1 + \chi_0)\zeta - 4]}{\zeta(\zeta - 1)(3 + 7\chi_0)}, \quad (\text{C10})$$

which reduces, in the case of a pure photon gas ($E_0 = 3P_0 V_0$) to

$$h = \frac{\zeta - 7}{6\zeta}. \quad (\text{C11})$$

The square of the sound speed can be expressed as

$$c_s^2 = \left. \frac{\partial P}{\partial \rho} \right|_T + \frac{T}{\rho^2} \left(\left. \frac{\partial P}{\partial T} \right|_{\rho} \right)^2. \quad (\text{C12})$$

with $E = E_{\text{rad}} = \frac{4\sigma}{c} T^4 V$ and $P = P_{\text{rad}} = \frac{4\sigma}{3c} T^4$, we have

$$\left. \frac{\partial P}{\partial \rho} \right|_T = 0 \quad (\text{C13})$$

and

$$c_s^2 = \frac{4}{3} PV, \quad (\text{C14})$$

which is a particular case of $c_s^2 = \gamma PV$ for $\gamma = 4/3$. The Mach number becomes

$$M^2 = \frac{(D - u)^2}{c_s^2} = \frac{3}{2(\zeta - 1)} \frac{[(1 + \chi_0)\zeta - 4]}{[(1 + 2\chi_0)\zeta - 1]} \quad (\text{C15})$$

and reduces, in the case of a pure photon gas ($E_0 = 3P_0 V_0$), to

$$M^2 = \frac{6}{7\zeta - 1}, \quad (\text{C16})$$

and the critical parameter is

$$h_c = \frac{1 - (\zeta + 1)M^2}{1 - (\zeta - 1)M^2} = \frac{(\zeta - 7)[\zeta(\chi_0 - 1) - 2]}{(\zeta - 1)[\zeta(5 + 7\chi_0) - 14]}, \quad (\text{C17})$$

which reduces, in the case of a pure photon gas, to

$$h_c = \frac{\zeta - 7}{13\zeta - 7}. \quad (\text{C18})$$

Therefore, $h > h_c$ implies that $\zeta < \zeta_t$, where ζ_t is a positive real solution of the second-order equation

$$2(1 + 2\chi_0)\zeta^2 - 7(1 + \chi_0)\zeta + 14 = 0. \quad (\text{C19})$$

As can be seen in Fig. 26, in the range $0 < \chi_0 < 3$, which includes the values of our EOS model (see Table II), Eq. (C19) has no real solution (for $\chi_0 = 3$, the only real solution is $\zeta = 1$). Therefore, we always have $h < h_c$, which means that when the radiation dominates, the system is always stable (see Fig. 27).

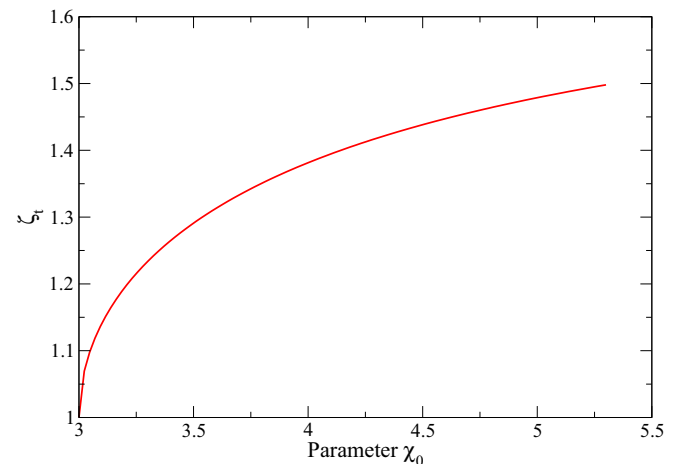


FIG. 26. Value of ζ_t as a function of parameter χ_0 .

TABLE II. Values of $\chi_0 = \frac{E_0}{\rho_0 V_0}$ for the different elements considered in the present paper.

Element	Value of χ_0
C	1.85
Al	1.99
Si	1.95
Nb	2.02

Of course, the case $\chi_0 = 3$, corresponding to a pure photon gas, is not physical. Naturally, shock waves cannot exist in a photon gas because a shock wave is a nonlinear flow. Nonlinear hydrodynamic equations used by D'yakov and Kontorovich can describe shock fronts. To consider shock fronts in a photon gas, one needs a significant photon-photon scattering, a nonlinear QED effect, which is only possible if the corresponding electromagnetic field strength exceeds the Schwinger limit [68–70], allowing the interacting photons to produce virtual electron-positron pairs, which means that the temperature of the photon gas must be in MeV range and that the post-shock pressure should exceed $\approx 10^{10}$ Gbar,

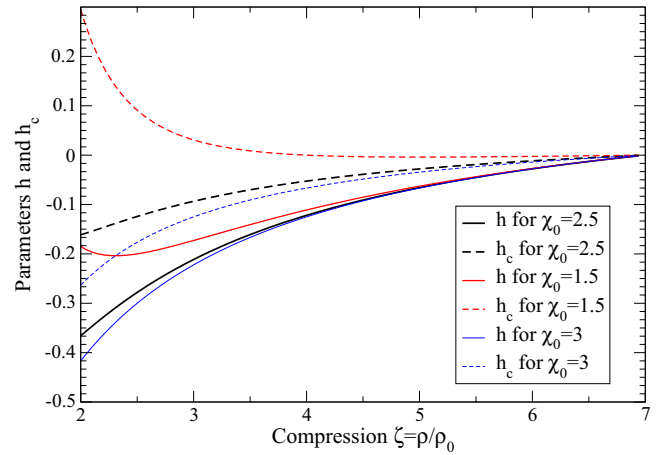


FIG. 27. Variation of parameters h and h_c versus compression $\zeta = \rho/\rho_0$ for three different values of parameter χ_0 : 1.5, 2.5, and 3. The conditions in which the photon gas is the dominant contribution to the EOS in the present work starts at $\zeta \approx 5$.

i.e., 10^{15} GPa, orders of magnitude above the pressure range studied in the present work.

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