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Irreversible thermodynamics of overdriven shocks in solids

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An isotropic solid, capable of transporting heat and of undergoing dissipative plastic flow, is treated. The shock is assumed to be a steady wave, and any phase changes or macroscopic inhomogeneities which might be induced by the shock are neglected. Under these conditions it is established that for an overdriven shock, no solution is possible without heat transport, and when the heat transport is governed by the steady conduction equation, no solution is possible without plastic dissipation as well. Upper and lower bounds are established for the thermodynamic variables, namely the shear stress, temperature, entropy, plastic strain, and heat flux, as functions of compression through the shock.

I. INTRODUCTION

We have recently discussed the irreversible-thermodynamic theory of flow processes in solids.[1–3] The processes considered include simultaneous elastic strain and plastic flow, where plastic flow is any dissipative rearrangement of the atoms in a solid. The theory is expressed in three coupled subsets of equations: the continuum-mechanic equations for conservation of mass, momentum, and energy; the thermoelastic equations which relate variations in the elastic strains, stresses, entropy, temperature, and so on; the thermoplastic equations which define plastic flow and specify the entropy generation. When the thermoelastic coefficients, which are the stress-strain coefficients, the anisotropic Grüneisen parameters, and the heat capacity at constant elastic configuration, and the plastic constitutive relations are known, the equations can be integrated from initial conditions to find a general flow process of a solid.

When applied to the problem of weak shocks in solids,[4] this work provides an improvement in the description of the shock process in two ways: Entropy terms in the stress equations are properly included (instead of using Hooke's law) and the entropy production is properly expressed in terms of plastic flow (instead of using viscous fluid dissipation).[1] Further, the theory can be used to determine the plastic flow behavior in the weak-shock process, from measurements of the shock profiles and the polycrystalline thermoelastic coefficients.[2] Finally, a solid-state Hugoniot theory has been given for the first time, from which it is possible to determine accurate equation-of-state data from weak shocks in solids.[3]

For overdriven shocks,[4] there is very little experimental information about the nature of the shock process. The shock is generally too fast to be experimentally resolved; an experimental upper limit for the rise time for shocks of several hundred kbar in several metals is 3 ns.[5] However, by applying the same principles we have previously used in the weak-shock theory, it is possible to learn a great deal about the process of overdriven shocks in solids, even without knowing details of the plastic constitutive behavior of the material. The purpose of the present paper is to develop this theory of overdriven shocks in solids.

The solid material is assumed to be isotropic, according to the definition of Ref. 1, and capable of transporting heat and of undergoing dissipative plastic flow. Polycrystalline effects are neglected; some justification for this is given in the Appendix. Shock-induced phase transitions, such as melting and other structural changes, and shock-induced macroscopic inhomogeneities, such as cracks and local hot spots, are also neglected. The shock is assumed to be a steady wave. The theory has been developed with application to polycrystalline metals in mind, but it might be valid for some nonmetals as well.

II. RAYLEIGH-LINE EQUATIONS

A. The conservation equations

The shock is a plane wave which propagates in the x direction; y and z are equivalent transverse directions. Lateral edge effects are eliminated by specifying that there is no material motion in transverse directions. Mass elements of the material are planar slabs of infinitesimal thickness, normal to the propagation direction. The Lagrangian coordinate of each mass element is X, which is equal to the laboratory coordinate x of the mass element before the shock arrives, i.e., at the time $t=-\infty$. The mechanic and thermodynamic properties of each mass element are functions of t, so for the whole material these properties are functions of X and t. The density is ρ, the volume per unit mass is $V=\rho^{-1}$, the material velocity is v, compressive stresses in the normal and transverse directions are, respectively, σ and $\sigma-2\tau$, so the shear stress is τ. Quantities in the initial state (before the shock) are denoted by subscript a, and $\epsilon=1-V/V_a$ measures the total compression from the initial state. The heat flux is J.

The shock is assumed to be a steady wave, moving at constant velocity D. The steady-wave condition is that any property $F(X,t)$ depends only on the Lagrangian steady-wave variable $Z=X-Dt$: $F(X,t)=F(Z)$. Equivalently, with $z=x-Dt$ the laboratory steady-wave variable, the condition is $F(x,t)=F(z)$. The two variables are related by

$$dZ=(\rho/\rho_a)dz \ . \tag{1}$$

Because of the steady-wave condition, the entire space and time dependence of any function $F(\epsilon)$ on the Rayleigh line is specified by a single variable.

The initial conditions are that the stresses, the material velocity, and the heat flux are zero in the state ahead of the shock,

$$\sigma_a=\tau_a=v_a=J_a=0 \ . \tag{2}$$

First integrals of the equations for conservation of mass and conservation of momentum are, respectively,

$$\epsilon=v/D \ , \tag{3}$$

$$\sigma=\rho_a D v \ . \tag{4}$$

The Rayleigh line is the $\sigma(\epsilon)$ relation through the shock process; from (3) and (4) this is

$$\sigma=\rho_a D^2\epsilon \ . \tag{5}$$

Since the transverse stresses do no work, the incremental center-of-mass work done on the material is $dW=-\sigma dV$ per unit mass. The incremental heat transferred to the material is dQ per unit mass, so conservation of energy requires

$$dU=-\sigma dV+dQ \ . \tag{6}$$

This equation includes arbitrary entropy generation, corresponding to whatever part of the work dW is dissipated, in addition to the entropy generation due to heat flow. It is convenient to eliminate Q for J, because J is the function customarily related to the material heat-transport properties. For a steady wave the continuity equation is simply $dQ=dJ/\rho_a D$, and the energy is integrated on the Rayleigh line to give

$$U-U_a=\tfrac{1}{2}D^2\epsilon^2+J/\rho_a D \ . \tag{7}$$

B. The thermodynamic equations

The thermodynamic equations include both thermoelastic and thermoplastic subsets; the derivation proceeds as follows.[1] Total symmetric strain measures may be taken as $\dot{\epsilon}_{ij}=\frac{1}{2}(v_{ij}+v_{ji})$, where v_{ij} are velocity gradients; ϵ_{ij} increments are composed of elastic and plastic parts: $d\epsilon_{ij}=d\epsilon_{ij}^e+d\epsilon_{ij}^p$; the $d\epsilon_{ij}^e$ are related in the usual way to variations in stresses, energy, entropy, and so on, and $d\epsilon_{ij}^p$ are related to plastic constitutive behavior and to the entropy production. Note that all these thermodynamic equations are Lagrangian, in that they relate various properties of a given mass element. In the present case of plane-wave motion there are only four independent strain variables: $d\epsilon_{xx}^e$, $d\epsilon_{yy}^e=d\epsilon_{zz}^e$, $d\epsilon_{xx}^p$, and $d\epsilon_{yy}^p=d\epsilon_{zz}^p$. The boundary condition of no transverse motion requires $d\epsilon_{yy}=d\epsilon_{zz}=0$, and the assumption that the plastic flow is volume conserving means $d\epsilon_{xx}^p+2d\epsilon_{yy}^p=0$. There remain only two independent strain variables, which may be taken as the total compression ϵ and the plastic strain ψ, where $d\psi=-d\epsilon_{xx}^p$. It is also convenient on occasion to use V or ρ in place of ϵ.

The thermoelastic equations may be derived in complete tensor form, appropriate for arbitrary elastic strains, by taking $d\epsilon_{ij}^e$ and dS as independent variables, where S is the entropy per unit mass. These equations may then be simplified for the present geometry. The results for the energy U, the stresses σ and τ, and the temperature T are the following[1]:

$$dU=TdS-\sigma dV-2V\tau d\psi \ , \tag{8}$$

$$d\sigma=\rho\gamma_1 TdS-B_{11}d\ln V-(B_{11}-B_{12})d\psi \ , \tag{9}$$

$$d\tau=\tfrac{1}{2}\rho(\gamma_1-\gamma_2)TdS-\tfrac{1}{2}(B_{11}-B_{21})d\ln V -\tfrac{1}{2}(B_{11}+\tfrac{1}{2}B_{22}+\tfrac{1}{2}B_{23}-B_{12}-B_{21})d\psi \ , \tag{10}$$

$$dT=C_\eta^{-1}TdS-T\gamma_1 d\ln V-T(\gamma_1-\gamma_2)d\psi \ . \tag{11}$$

Here the Voigt indices are $1=xx$, $2=yy$, $3=zz$. $B_{\alpha\beta}$ are the adiabatic stress-strain coefficients, γ_β are the anisotropic Grüneisen parameters, and C_η is the heat capacity at constant elastic configuration.[6] We also have to specify the entropy production. There are two sources in the present theory: dQ contributes to TdS, and also the plastic work $dW^p=2V\tau d\psi$, which is assumed to be totally dissipative,

$$TdS=dJ/\rho_a D+2V\tau d\psi \ . \tag{12}$$

Concerning the energy equation, we note that the continuum mechanic form (6) and the thermodynamic form (8) are the same when (12) for TdS is used. Because we have used the entropy as an independent variable, the energy equation is not coupled to the other thermodynamic equations (9)–(12), and so the energy equation does not have to be solved simultaneously with them.

To complete the description of the process, two more equations describing dynamic response characteristics of the material are needed. The plastic constitutive behavior is expressible as a dependence of the stress which drives the plastic flow, namely the shear stress τ, on the plastic strain and strain rate and on the thermodynamic state, approximately

$$\tau=\tau(\psi,\dot{\psi},V,S) \ . \tag{13}$$

The heat transport behavior relates the heat current J to the temperature gradient and other variables

$$J=J(\text{grad}\, T,V,S,\ldots) \ . \tag{14}$$

The complete set of Rayleigh-line equations is then (5) together with (9)–(14). We assume the thermoelastic coefficients $B_{\alpha\beta},\gamma_\beta,C_\eta$ are known as functions of the thermoelastic state. There are then seven coupled Rayleigh-line equations in the seven variables: σ,τ,T,S,ψ,J, and one space-time variable, z, for example. These equations are in principle solvable for the shock process. On the other hand, if one of the Rayleigh-line variables were known from experiment, e.g., $z(\epsilon)$, or $T(\epsilon)$, or for example $v(t)$ at a fixed X, then these equations can in principle be used to determine the plastic constitutive relation (13) through the shock. An alternate point of view, which we pursue in the following because there is no experimental data on the Rayleigh-line variables, and because the plastic constitutive behavior in overdriven shocks is entirely unknown, is to omit the last two equations of the set, and to study Eqs. (5) and (9)–(12), which are five equations in the six variables σ,τ,T,S,ψ,J. Following this, some information on the heat transport mechanism will be used to extend the study to the space-time dependence of the process.

III. THEOREMS ON THE SHOCK PROCESS

A. Necessity of heat transport

Theorem 1. For an overdriven shock in a solid, no solution is possible without heat transport.

The proof does not depend on the mechanism of heat transport. Heat transport is needed at the beginning of the shock, to bring σ up to the Rayleigh line, as shown in Fig. 1. The elastic line corresponds to adiabatic ($dS=0$) uniaxial elastic compression of the material under plane-wave boundary conditions (no transverse motion). The slope of this line at $\epsilon=0$ is $\rho_a c_l^2$, where c_l is the longitudinal sound velocity in state a. The elastic precursor velocity is $c_p \geq c_l$, where c_p can be greater than c_l by only very small finite-strain corrections. The definition of an overdriven shock is $D>c_p$, the slope of the Rayleigh line for a steady-wave shock is $\rho_a D^2$, so for an overdriven shock the Rayleigh line is steeper than the elastic line, as shown in Fig. 1. If plastic flow takes place in the small-ϵ region, it can only reduce σ below the elastic line at small ϵ. Therefore heat must be transported to the material in the initial stage of the shock.

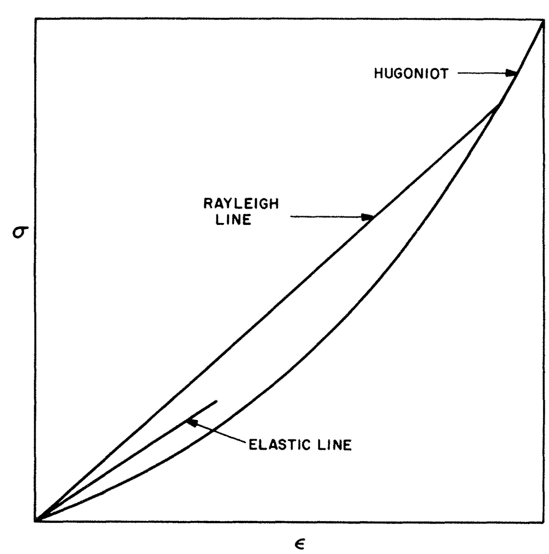

FIG. 1. Showing the proof of Theorem 1. The elastic line has a fixed slope of $\rho_a c_l^2$ at $\epsilon=0$; the Rayleigh line has slope $\rho_a D^2$ which increases with shock velocity D.

The proof may be shown directly from the Rayleigh-line equations. We set the heat transport to zero: $dJ=0$. Then from (12), $TdS=0$ at state a, since $\tau_a=0$. Also at state a, $\rho=\rho_a$, $B_{11}=\rho_a c_l^2$, $B_{11}-B_{12}=2G$, where G is the adiabatic shear modulus, so (9) at state a is

$$d\sigma=\rho_a c_l^2 d\epsilon-2Gd\psi \ .$$

Differentiating the Rayleigh-line equation (5) for a fixed D gives

$$d\sigma=\rho_a D^2 d\epsilon \ .$$

Since $d\psi\geq 0$ by definition, no solution is possible when $D>c_l$. When heat transport is included, $dJ>0$ and a solution is possible.

B. Family of partial solutions

Consider a given material with specified properties and a fixed shock strength corresponding to a shock velocity D. The state behind the shock is the thermodynamic equilibrium Hugoniot state, denoted by subscript H, where the Rayleigh line reaches the Hugoniot at ϵ_H. The thermodynamic variables have the values $\sigma_H,\tau_H,T_H,S_H,\psi_H$, and because of equilibrium the heat current vanishes:

$$J_H=0 \ . \tag{15}$$

Because the shock is a continuous process, the Rayleigh-line solution is continuous, i.e., all the variables are continuous functions of ϵ for $0\leq\epsilon\leq\epsilon_H$.

We define a partial solution as a set of six functions $\sigma(\epsilon)$, $\tau(\epsilon)$, $T(\epsilon)$, $S(\epsilon)$, $\psi(\epsilon)$, and $J(\epsilon)$ which are continuous on $0\leq\epsilon\leq\epsilon_H$, which take on the correct values at $\epsilon=0$ and ϵ_H, and which satisfy the five Rayleigh-line equations (5) and (9)–(12). A partial solution can be constructed by taking any function for one of the variables, for example $S(\epsilon)$, which is continuous and which takes on the correct values at $\epsilon=0$ and ϵ_H, and by solving the five Rayleigh-line equations for the other five functions. Given $S(\epsilon)$, solution for the other five functions is unique, because for the tetragonal symmetry of the material under plane-wave compression there are three independent thermoelastic state variables, which can be taken as S,ϵ,σ, and $\sigma(\epsilon)$ is fixed by Eq. (5). Because one function of a partial solution is arbitrary, the family of partial solutions is infinite. Among these, many will be unacceptable on simple physical grounds, as we will see shortly; among the physically acceptable partial solutions, one is the correct solution for the material under consideration.

It is possible to establish an important ordering of the partial solutions. Starting from one partial solution, we generate another one infinitesimally removed by adding to $S(\epsilon)$ an increment $\delta S(\epsilon)$, which is continuous and which does not change sign on $0\leq\epsilon\leq\epsilon_H$, and which vanishes at $\epsilon=0$ and at ϵ_H. From one given partial solution, all partial solutions can be generated in this way. Functional relations among the variations $\delta S(\epsilon)$, $\delta T(\epsilon)$, and so on, at a fixed value of ϵ, can be found from Eqs. (5) and (9)–(12) evaluated at $\delta\epsilon=0$:

$$\delta\sigma=0 \ , \tag{16}$$

$$\delta\sigma=\rho\gamma_1 T\delta S-(B_{11}-B_{12})\delta\psi \ , \tag{17}$$

$$\delta\tau=\tfrac{1}{2}\rho(\gamma_1-\gamma_2)T\delta S-\tfrac{1}{2}(B_{11}+\tfrac{1}{2}B_{22}+\tfrac{1}{2}B_{23}-B_{12}-B_{21})\delta\psi \ , \tag{18}$$

$$\delta T=C_\eta^{-1}T\delta S-T(\gamma_1-\gamma_2)\delta\psi \ , \tag{19}$$

$$T\delta S=\delta J/\rho_a D+2V\tau\delta\psi \ . \tag{20}$$

These relations will eventually be useful in establishing bounds for the Rayleigh-line solution throughout the shock.

The coefficients in these equations are complicated, but a consistent use of the small-anisotropy expansion is sufficient to determine the relative signs of the variations $\delta S(\epsilon)$, $\delta T(\epsilon)$, and so on. The small-anisotropy expansion is defined as follows[1]: Throughout the shock process, the shear stress τ should be small compared to the shear modulus G, so any thermodynamic coefficient $f=f(\epsilon,S,\tau)$ can be expanded in powers of τ/G at constant ϵ,S:

$$f(\epsilon,S,\tau)=f(\epsilon,S,0)+(\text{coefficient})(\tau/G)+\cdots \ . \tag{21}$$

For the needed coefficients we write explicitly the leading term in the expansion, which is defined in isotropic thermodynamic space ($\tau=0$), and denote by $+\cdots$ all terms of relative order τ/G and higher:

$$\begin{aligned}
&\gamma_1=\gamma+\cdots \ ,\\
&\gamma_2=\gamma+\cdots \ ,\\
&B_{11}=B+\tfrac{4}{3}G+\cdots \ ,\\
&B_{11}-B_{12}=2G+\cdots \ ,\\
&\tfrac{1}{2}(B_{11}+\tfrac{1}{2}B_{22}+\tfrac{1}{2}B_{23}-B_{12}-B_{21})=\tfrac{3}{2}G+\cdots \ ,\\
&C_\eta=C_V+\cdots \ ,
\end{aligned} \tag{22}$$

where γ is the ordinary (isotropic) Grüneisen parameter, B is the adiabatic bulk modulus, and C_V is the heat capacity at constant volume.

Relative signs of the variations δS, δT, and so on, are given by the leading order evaluation of Eqs. (16)–(20). In view of (16) and (17), the first term on the right of (18) may be neglected because it is of order τ/G times the second term. Also because $TC_V \lesssim VG$ for shocks in solids,[7] the second term on the right of (19) is $\lesssim(\tau/G)$ times the first term. Then to leading order the functional variations at fixed ϵ are related by

$$\delta\psi(\epsilon)=(\rho\gamma T/2G)\delta S(\epsilon) , \tag{23}$$

$$\delta T(\epsilon)=(T/C_V)\delta S(\epsilon) , \tag{24}$$

$$\delta J(\epsilon)=\rho_a DT\delta S(\epsilon) , \tag{25}$$

$$\delta\tau(\epsilon)=-\tfrac{3}{4}\rho\gamma T\delta S(\epsilon) . \tag{26}$$

Therefore, given any partial solution, functional variation to a new partial solution has $\delta S(\epsilon)$, $\delta T(\epsilon)$, $\delta\psi(\epsilon)$, $\delta J(\epsilon)$ of the same sign everywhere, and $\delta\tau(\epsilon)$ of the opposite sign everywhere. The next step is to introduce physical restrictions that will limit the range of partial solutions which are acceptable.

C. The minimum-τ partial solution

For a solid, τ cannot be negative during shock compression, hence $\tau=0$ is a lower bound for $\tau(\epsilon)$ on the Rayleigh line. We can construct a partial solution, the minimum-τ partial solution, by specifying $\tau(\epsilon)$ as follows: $\tau(\epsilon)=0$ for $0\le\epsilon\le\epsilon_H-\delta$, where δ is a positive infinitesimal, and $\tau(\epsilon)$ increases continuously to τ_H at ϵ_H. If we want to set $\tau_H=0$, i.e., to approximate the solid Hugoniot by a fluid Hugoniot, then the minimum-τ partial solution has $\tau(\epsilon)=0$ everywhere. Specifying $\tau(\epsilon)$ determines a partial solution, whose properties follow directly from Eqs. (5) and (9)–(12), and from the ordering of the family of partial solutions:

Theorem 2. The minimum-τ partial solution represents, in the region where $\tau(\epsilon)=0$, an inviscid fluid with heat transport, and it constitutes a bound for physically acceptable solutions, in which $T(\epsilon)$, $S(\epsilon)$, $\psi(\epsilon)$, $J(\epsilon)$ are all upper bounds.

The qualitative forms of $T(\epsilon)$ and $J(\epsilon)$ for the minimum-τ partial solution are shown in Fig. 2. The Rayleigh-line equations simplify in the region where $\tau=0$. The stress becomes an isotropic pressure P, and all the thermodynamic coefficients are evaluated at $\tau=0$, which is the state corresponding

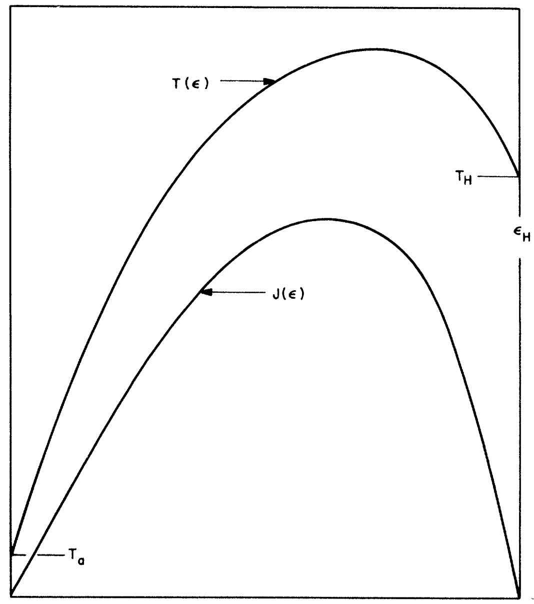

FIG. 2. Behavior of $T(\epsilon)$ and $J(\epsilon)$ on the Rayleigh line for an inviscid fluid with heat transport or a solid with $\tau(\epsilon)=0$.

to the leading terms in (22). Equation (10) is

$$0=-G(d\ln V+\tfrac{3}{2}d\psi) , \tag{27}$$

which allows $d\psi$ to be eliminated from the set. Equations (5), (9), (11), (12) then become

$$\sigma=P=\rho_a D^2\epsilon , \tag{28}$$

$$dP=\rho\gamma TdS+\rho V_a Bd\epsilon , \tag{29}$$

$$dT=\rho\gamma V_a Td\epsilon+C_V^{-1}TdS , \tag{30}$$

$$TdS=dJ/\rho_a D . \tag{31}$$

D. The minimum-ψ partial solution

The plastic strain must be nondecreasing by definition: $d\psi\ge 0$. Hence $\psi=0$ is a lower bound for $\psi(\epsilon)$ on the Rayleigh line. The condition $\psi=0$ represents the response of an elastic solid with heat transport and with infinite yield strength; we refer to this hypothetical material as a nonplastic solid. If we set $\psi(\epsilon)=0$ the Rayleigh-line equations can be solved. Figure 3 shows the behavior of $J(\epsilon)$ and $T(\epsilon)$ in this case: $J(\epsilon)$ has a maximum at some point ϵ_b, and $T(\epsilon)$ has a maximum at $\epsilon_d>\epsilon_b$. This solution is not a partial solution because the variables do not reach the Hugoniot values at ϵ_H; we find, in particular, $T(\epsilon_H)<T_H$ and $J(\epsilon_H)<0$.

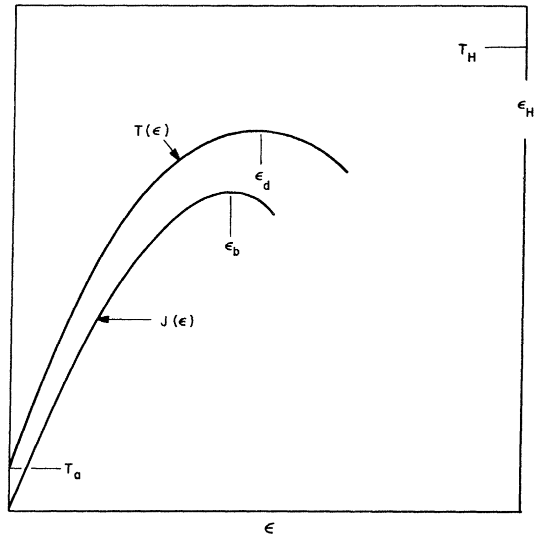

FIG. 3. Behavior of $T(\epsilon)$ and $J(\epsilon)$ on the Rayleigh line for a solid with heat transport and with $\psi=0$ (a nonplastic solid). $J(\epsilon)$ has a maximum at ϵ_b and $T(\epsilon)$ has a maximum at $\epsilon_d > \epsilon_b$.

In other words, the nonplastic solid does not possess a steady-wave shock solution. But we are only interested in this solution in the region $0 \leq \epsilon \leq \epsilon_d$; beyond this, one of the thermodynamic variables can be arbitrarily continued to the Hugoniot state, generating a partial solution. This partial solution, with $\psi(\epsilon)=0$ for $0 \leq \epsilon \leq \epsilon_d$, is called the minimum-$\psi$ partial solution. Properties which follow at once from Eqs. (5) and (9)–(12) and from the ordering of the family of partial solutions are the following.

Theorem 3. The minimum-ψ partial solution in the region where $\psi(\epsilon)=0$ represents a nonplastic solid, and constitutes a bound for physically acceptable solutions in which $T(\epsilon)$, $S(\epsilon)$, $J(\epsilon)$ are lower bounds and $\tau(\epsilon)$ is an upper bound.

The condition $d\psi=0$ simplifies the Rayleigh-line equations considerably. Combining (5) and (9) gives

$$\rho\gamma_1 TdS=(\rho_a D^2-\rho V_a B_{11})d\epsilon \ , \tag{32}$$

and (11) and (12) become

$$dT=\rho\gamma_1 V_a Td\epsilon+C_\eta^{-1}TdS, \tag{33}$$

$$TdS=dJ/\rho_a D \ . \tag{34}$$

These are three equations in $T(\epsilon)$, $S(\epsilon)$, $J(\epsilon)$. The equation for $\tau(\epsilon)$ is then uncoupled from the above set:

$$d\tau=\tfrac{1}{2}\rho(\gamma_1-\gamma_2)TdS+\tfrac{1}{2}\rho V_a(B_{11}-B_{12})d\epsilon \ . \tag{35}$$

E. Solutions continuous in space and time

To study the space and time dependence of the shock process, we need to know something about the dynamic response characteristics of the material. There is currently no sound basis for estimating plastic flow behavior under conditions of overdriven shocks. However, a respectable estimate of the heat transport mechanism can be made, and we will do this specifically for metals.

For an ordinary metal, solid, or liquid phase, undergoing a shock to the few Mbar range, the compression is about a factor of 2, and the temperature rises to the order of 10^4 K. These changes are mild for most metals, so the nature of the electron-phonon system in its simplest approximation is not significantly changed. We can still think of electrons carrying the heat, and being scattered by electrons and phonons. Further, if irreversible thermodynamics is approximately valid, the heat current should be given approximately by the steady conduction equation $J=-\kappa\,\mathrm{grad}T$.

Elementary solid-state theory for electronic conduction at high temperatures ($T \gtrsim$ Debye temperature) expresses the conductivity κ as[8–11]

$$\kappa=\tfrac{1}{3}Cv_F^2 t_e \ ,$$

where C is the electronic heat capacity per unit volume, v_F is the Fermi velocity, and t_e is the dominant electronic relaxation time. The electron-phonon relaxation time is $t_{ep} \sim 10^{-14}$ s at room temperature and should decrease through the shock approximately as T^{-1}. The electron-electron relaxation time is $T_{ee} \sim 10^{-12}$ s at room temperature and should decrease approximately as T^{-2}. Hence t_{ee} will become dominant at sufficiently strong shocks, but up to a few Mbar, t_{ep} should ordinarily be dominant. With t_{ep} as the electronic relaxation time, the above expression for κ has the following properties[8–11]: κ is independent of T, and κ has only a small density dependence of order ρ to ρ^2. So in the shocks under consideration, κ is roughly constant.

The thermodynamic variables σ, τ, T, S, ψ, J should be continuous single-valued functions of space and time through the shock, or what is equivalent, they should be continuous single-valued functions of z. This requirement leads to a condition on the behavior of $T(\epsilon)$ and $J(\epsilon)$, which we will derive. The heat-conduction equation for a steady plane wave is

$$J=-\kappa(\partial T/\partial x)_t=-\kappa(dT/dz) \ , \tag{36}$$

or with $d\epsilon > 0$,

$$J = -\kappa \frac{dT/d\epsilon}{dz/d\epsilon} . \quad (37)$$

For overdriven shocks, Theorem 1 implies $J(\epsilon)$ and $dT/d\epsilon$ are both positive at small ϵ. As ϵ increases Eq. (37) allows the following possibilities. If $dT/d\epsilon=0$ on a finite interval while $J(\epsilon)>0$, then $\epsilon(z)$ is discontinuous. If $dT/d\epsilon<0$ on a finite interval while $J(\epsilon)>0$, then $\epsilon(z)$ is double valued. If $J(\epsilon)=0$ on a finite interval while $dT/d\epsilon>0$, then $z(\epsilon)$ is undefined. If $J(\epsilon)<0$ on a finite interval while $dT/d\epsilon>0$, then $\epsilon(z)$ is double valued. All of these cases can be rejected, because if ϵ is discontinuous or double valued in z, then the thermodynamic variables are also discontinuous or double valued in z. Then either $J(\epsilon)$ and $dT/d\epsilon$ both remain positive on $0<\epsilon<\epsilon_H$ or else both are zero at some $\epsilon'<\epsilon_H$.

In fact, both $J(\epsilon)$ and $dT/d\epsilon$ must remain positive, as can be shown from the Rayleigh-line equations. In (11) the last term on the right is of order τ/G relative to the second term, so the sign of the last two terms together is the sign of the second term, from which it follows that $T(dS/d\epsilon)<0$ when $dT/d\epsilon \leq 0$. Then because $\tau(d\psi/d\epsilon)\geq 0$, (12) implies $dJ/d\epsilon<0$ when $dT/d\epsilon\leq 0$. Now suppose J and $dT/d\epsilon$ are zero at $\epsilon'<\epsilon_H$. Then if $dT/d\epsilon\leq 0$ all the way to ϵ_H, $dJ/d\epsilon<0$ all the way to ϵ_H, and $J(\epsilon_H)<0$, which violates the final condition (15). If instead $dT/d\epsilon\leq 0$ for $\epsilon'\leq\epsilon\leq\epsilon''$, where $\epsilon''<\epsilon_H$ and $dT/d\epsilon>0$ for a finite interval of $\epsilon>\epsilon''$, then $J(\epsilon)<0$ for a finite interval of $\epsilon>\epsilon''$ and $\epsilon(z)$ is double valued. Hence we have the following theorem.

Theorem 4. For an overdriven shock in a solid with heat conduction and dissipative plastic flow, a steady-wave solution continuous and single valued in z is possible only under the conditions $J(\epsilon)\geq 0$, $dT/d\epsilon\geq 0$, on $0\leq\epsilon, \leq\epsilon_H$, where either equality can hold on a sum of intervals whose total length is zero.

F. Bounds throughout the shock

It is now possible to construct upper and lower bounds for the temperature through the shock process. The construction is shown in Fig. 4, where the curves are those computed for a 0.8 Mbar shock in 2024 Al, with the approximation $\tau_H=0$. The inviscid fluid curve is the $\tau=0$ partial solution [Theorem 2 and Eqs. (27)–(31)]; it reaches T_H at ϵ^* and so, because $dT/d\epsilon\geq 0$ for $0<\epsilon<\epsilon_H$ by

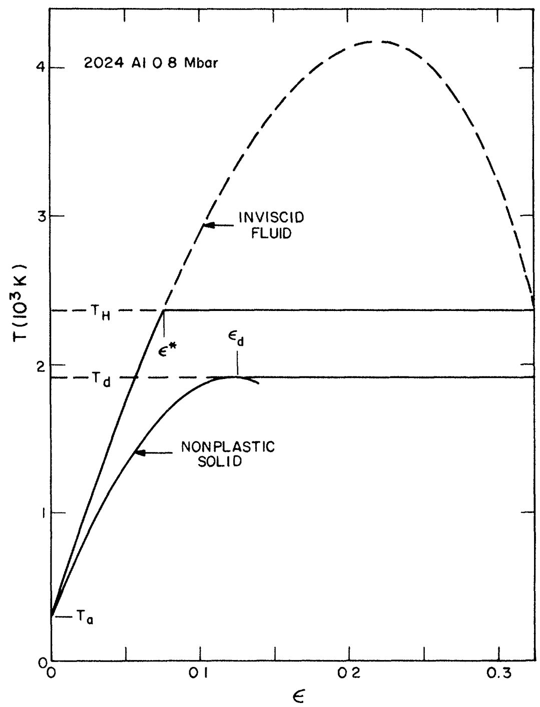

FIG. 4. Solid lines show upper and lower bounds for $T(\epsilon)$ on the Rayleigh line. Curves plotted are for a 0.8 Mbar shock in 2024 Al, where $\tau_H=0$ has been taken for approximation (ϵ_H = 0.324, T_H=2365 K).

Theorem 4, an upper bound for $T(\epsilon)$ on $\epsilon^* \leq\epsilon\leq\epsilon_H$ is T_H. The nonplastic solid curve is the $\psi=0$ partial solution [Theorem 3 and Eqs. (32)–(35)]; it has a maximum of T_d at ϵ_d and so, because $dT/d\epsilon\geq 0$ for $0<\epsilon<\epsilon_H$, a lower bound for $T(\epsilon)$ on $\epsilon_d\leq\epsilon\leq\epsilon_H$ is T_d.

For the real shock process in a solid with heat conduction and dissipative plastic flow, the $T(\epsilon)$ curve must lie within the bounds illustrated in Fig. 4, must be a nondecreasing function of ϵ, and must reach T_H at ϵ_H. Further, with the upper bound for $T(\epsilon)$ prescribed as in Fig. 4, a partial solution of the Rayleigh-line equations can be found, in which $S(\epsilon)$, $\psi(\epsilon)$, $J(\epsilon)$ are upper bounds and $\tau(\epsilon)$ is a lower bound. Also for the lower bound $T(\epsilon)$ shown in Fig. 4, another partial solution can be found, in which $S(\epsilon)$, $\psi(\epsilon)$, $J(\epsilon)$ are lower bounds and $\tau(\epsilon)$ is an upper bound. This gives a great deal of information about the shock process.

G. Necessity of plastic dissipation

With reference to Fig. 4 and with $\tau_H=0$ for approximation, we consider the possibility that the inviscid fluid solution for $T(\epsilon)$ remains less than T_H for $0 \leq \epsilon < \epsilon_H$ and reaches T_H at ϵ_H. In his classic paper on shocks in gases, Rayleigh[12] has shown that this is the case for sufficiently weak shocks, but not for shocks stronger than a certain limit. We express this limit in the form $D = (1+x)c_B$, where c_B is the "bulk sound velocity," given by $\rho c_B^2 = B$. For dense systems such as $\rho_a \gtrsim 1$ g/cm^3, and corresponding values of γ_a and C_V, we find $x \sim 10^{-2}$. This value of D is certainly less than the longitudinal sound velocity, so we conclude that for overdriven shocks the inviscid fluid curve of $T(\epsilon)$ passes above T_H at some $\epsilon^* < \epsilon_H$, as shown in Fig. 4. It is therefore possible to establish the following theorem.

Theorem 5. For an overdriven shock in a solid with heat conduction, no solution is possible without plastic dissipation.

The theorem is most easily proved from Fig. 4. The inviscid fluid $T(\epsilon)$ corresponds to $\tau = 0$; therefore, in order to have $T(\epsilon) \leq T_H$ for $\epsilon > \epsilon^*$, we must have $\tau(\epsilon) > 0$ for $\epsilon > \epsilon^*$. The nonplastic solid $T(\epsilon)$ corresponds to $\psi = 0$; therefore, in order that $T(\epsilon) \geq T_d$ for $\epsilon > \epsilon_d$, we must have $\psi(\epsilon) > 0$ for $\epsilon > \epsilon_d$. Thus in the last part of the shock process, for $\epsilon > \epsilon^*$ and $\epsilon > \epsilon_d$, the plastic dissipation $dW^p = 2V\tau d\psi$ is greater than zero.

This result is approximately the counterpart for solids of Rayleigh's theorem[12] for viscous heat-conducting gases. Physically it arises because the heat which must be transported to the initial region of an overdriven shock, in order to bring σ up to the Rayleigh line according to Theorem 1, has to be generated by plastic dissipation in the later stage of the shock.

IV. SUMMARY AND DISCUSSION

We have studied the irreversible thermodynamic process of overdriven shocks in an isotropic solid with heat transport and dissipative plastic flow. Shock-induced macroscopic inhomogeneities and shock-induced phase changes are not considered. The theory developed is expected to apply to polycrystalline metals, and possibly to ductile nonmetals as well. Arguments can be given for the neglect of polycrystalline effects (the Appendix), but more experimental information on this question is needed.

Some comments can be made concerning the steady-wave assumption. When a shock is initiated, for example by a plate impact, the wave front presumably evolves as it moves. The assumption is that it approaches a steady wave (evolution approaches zero), and that for all practical purposes the real shock is well approximated by the limiting steady wave, after a distance of travel of many shock widths. The steady-wave assumption does not hold for weak shocks in solids[2,3] because the elastic precursor travels faster than the plastic wave and the entire shock continues to spread indefinitely. Also, for overdriven shocks a phase change could split the wave into two components traveling at different velocities. Obviously, then, the steady-wave assumption implies some restrictions on the dynamic response of a material. We note that heat transport according to the steady conduction equation is compatible with a steady wave.

The concept of the family of partial solutions is quite useful in analyzing the shock process because these solutions depend only on the best-known material properties, namely, the thermoelastic coefficients. For a given material, with thermoelastic coefficients known as functions of the thermoelastic state, the family contains all continuous solutions with the proper initial and final values, which are consistent with the thermoelastic coefficients and consistent with arbitrary (unspecified) dynamic response properties. Members of the family are ordered by observing that given a partial solution functional variation leads to a new partial solution with $\delta S(\epsilon)$, $\delta T(\epsilon)$, $\delta\psi(\epsilon)$, $\delta J(\epsilon)$ of the same sign everywhere, and $\delta\tau(\epsilon)$ of the opposite sign everywhere. Then because τ must be non-negative, $\tau(\epsilon) = 0$ defines a unique partial solution which gives upper bounds for $S(\epsilon)$, $T(\epsilon)$, $\psi(\epsilon)$, $J(\epsilon)$ (Theorem 2). And because ψ must be non-negative, $\psi(\epsilon) = 0$ defines a partial solution, unique up to ϵ_d where $dT/d\epsilon = 0$, which gives lower bounds for $S(\epsilon)$, $T(\epsilon)$, $\psi(\epsilon)$, $J(\epsilon)$, and an upper bound for $\tau(\epsilon)$, for $0 \leq \epsilon \leq \epsilon_d$ (Theorem 3). Further, the condition that the solution be continuous and single valued in z, coupled with the steady heat-conduction equation, requires $J(\epsilon)$ to be non-negative and $T(\epsilon)$ to be a nondecreasing function of ϵ (Theorem 4). This theorem then narrows the bounds on $T(\epsilon)$ and on the other variables as well (Fig. 4). Finally, it is established that for an overdriven shock in a solid no solution is possible without the operation of *both* dissipative mechanisms, heat transport and plastic flow (Theorems 1 and 5).

An observation is in order on the use of thermodynamics in the theory of shocks. In the present work, irreversible thermodynamics is assumed valid; this means thermodynamic functions are defined throughout the shock, and they are related by irreversible-thermodynamic relations. It is then possible to solve for, or at least to estimate, the space and time dependence of the shock process, and from this solution it is possible to determine whether or not irreversible thermodynamics is in fact valid. We will pursue this line of investigation in the future. In the following paper, the present theory is used as basis for numerical calculations for some representative metals, and it is found that the Rayleigh-line solution is narrowly bounded and the nature of the shock process is revealed in some detail.

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APPENDIX: POLYCRYSTALLINE EFFECTS

The question is, for overdriven shocks in solids, is the shock width (or rise time) influenced by polycrystalline effects; more specifically, does the polycrystal structure give rise to a significant dissipation in the shock process. Such dissipation could result if the shock velocity is different in different crystallographic directions and if the shock thickness is small compared to the grain size. Then in any two neighboring grains of different orientation, the shock will move faster in one and will transfer energy sideways to the other grain ahead of the shock front there; this is dissipative, and it broadens the shock front. We note that different shock velocities in different crystal directions can result if there is a noticeable shear stress in the shocked state, and especially if that shear stress is different for the different directions. On the other hand, if the Hugoniot shear stress is insignificant for shocks in all crystal directions, and if the shock is a steady wave, then the Hugoniot lies in isotropic thermodynamic space (stress system is isotropic pressure) and the shock velocity must also be isotropic.

As for experimental data, there is very little to help resolve the question. Grains in metals range nominally from 10^{-3} to 10^{-2} cm. According to the present theory, the width of overdriven shocks in metals is of order 10^{-6} cm, so the shock thickness is small compared to the grain size. The same should be true for any nonmetals to which the present theory might apply. For very weak shocks in NaCl ($3-15$ kbar), a large difference in plastic wave velocities in different crystal directions has been observed.[13] This has been explained by attributing the plastic flow entirely to primary slip.[14] For stronger shocks, driving higher order slip, dependence on crystal orientation is expected to become weaker. Shock velocity-particle velocity measurements for NaCl in different crystal directions all lie on the same curve up to 230 kbar (Ref. 15); a phase change which begins at 230 kbar introduces effects with which we are not concerned here. This result suggests that polycrystal effects should not be important in NaCl up to 230 kbar. For metals we might speculate that $\tau_H << \sigma_H$ for shocks in the Mbar range, so that shock velocity is insensitive to crystal direction and polycrystal effects are correspondingly negligible. Any experimental information which bears on this question would be welcome in the future.

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