Discontinuity Waves, Shock Formation and Critical Temperature in Crystals

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The propagation of discontinuity waves in a rigid heat conductor at low temperatures is studied by using a generalized non-linear Maxwell–Cattaneo equation developed in the framework of extended thermodynamics. The critical time (i.e., the instant in which a shock wave formation occurs) is evaluated in both cases of infinite and finite heat conductivity. The critical temperature \( \theta_c \), pointed out in our previous papers concerning the propagation of shock and simple waves, once more plays an important role: in fact, now it determines two different regimes for the wave propagation and this phenomenon, from a mathematical point of view, is related to the loss of the genuine non-linearity when \( \theta = \tilde{\theta} \). In the last sections some numerical results are given and a brief analysis about the evolution of a possible initial wave profile is performed.

1. INTRODUCTION

In some previous papers [1–3] the behaviour of a temperature pulse propagating in a solid was investigated, using a generalized non-linear Cattaneo model [4, 5] developed in the framework of extended thermodynamics [6]. In particular, in [1, 2], on the ground of the shock wave theory, it was proved the existence of a critical temperature \( \tilde{\theta} \), characteristic of the material, such that the nature of the shock changes: in fact, if the unperturbed temperature \( \theta_o \) is less than \( \tilde{\theta} \) the temperature \( \theta_1 \) behind the shock wave front must be such that \( \theta_1 > \theta_o \) (hot shock) and, vice versa, if \( \theta_o > \tilde{\theta} \) the contrary happens, i.e., \( \theta_1 < \theta_o \) (cold shock). By applying these results to some highly pure dielectric crystals, as NaF, Bi, \(^3\)He, and \(^4\)He, it was found that the temperature \( \tilde{\theta} \) is very close to the experimental temperature at which the second sound is clearly seen in these crystals [1].
In [3], solutions of simple wave type are found to describe the shape change of the pulse initially given by a gaussian function. Also in that framework the characteristic temperature plays an important role: the shape change of the propagating wave depends again on $\tilde{\theta}$, having now three different wave forms related to the unperturbed temperature and to the initial wave amplitude.

In the present paper we reconsider the problem concerning the propagation of discontinuity waves (acceleration waves in the language of continuum mechanics), first studied in [5, 7], to underline, once more, the fundamental role of the critical temperature $\bar{\theta}$: we prove, also in this framework, the existence of this temperature that determines two different regimes for the discontinuity wave propagation. From a mathematical point of view, this happens because the genuine non-linearity condition is lost when $\theta = \bar{\theta}$. The assumption about an initial discontinuity wave is justified by the fact that the pulse shape characterizing the rise of the temperature during the action of a thermal generator on a face of a crystal can be considered regular but its derivative changes very quickly since the phenomenon is about a few microseconds in duration. So, it seems to us that a discontinuity wave would be able to represent the initial temperature pulse even better than a simple wave (see [3]) if the thermal generator is very fast in the “on” and “off” states.

It must also be underlined that, at a difference from the papers [1–3], now the thermal conductivity is not assumed infinite but, on the ground of the experimental data, it depends on the temperature and so our numerical simulations acquire more reliability. Finally, we recall that in the last years this research area has interested many authors and in the papers [8–16] the reader can find a review of many problems concerning the propagation of a thermal pulse in a solid.

2. THE RIGID CONDUCTOR MODEL

In [1–3] the following non-linear system describing the heat propagation in a rigid conductor has been used

$$\rho \partial_t e + \text{div} \mathbf{q} = 0,$$

$$\partial_t (\alpha \mathbf{q}) + \text{grad} \nu = -\frac{\nu'}{\kappa} \mathbf{q}.$$

Here the prime is the derivative with respect to the temperature $\theta$, $\rho$ is the (constant) mass density, $e$ the internal energy, $\mathbf{q}$ the heat flux vector, $\kappa$ the heat conductivity (which may depend on $\theta$) and $\alpha, \nu$ are constitutive
scalars depending on $\theta$ and related to the second sound velocity $U_E \equiv U_E(\theta)$ by means of the following relations [2],

$$\nu = \int \frac{U_E(\theta)}{\theta} \sqrt{c_v(\theta)} \, d\theta, \quad \alpha = \frac{1}{\rho \theta U_E(\theta) \sqrt{c_v(\theta)}},$$

where $c_v(\theta) = c' = \epsilon \theta^3 > 0 \ (\epsilon = \text{constant})$ is the specific heat for crystals at low temperatures and $U_E$ is given by the following empirical equation [17],

$$U_E^2 = \frac{1}{A + B \theta^n}$$

fitting very well the values obtained from experiments for NaF [18] and Bi [19] crystals. Values of the quantities $A$, $B$, and $n$ in (4) are

\[\begin{align*}
n &= 3.10, & A &= 9.09 \cdot 10^{-12}, & B &= 2.22 \cdot 10^{-15} \\
& & 10 \text{ K} \leq \theta \leq 18.5 \text{ K} \ (\text{NaF}), & & & \\
n &= 3.75, & A &= 9.07 \cdot 10^{-11}, & B &= 7.58 \cdot 10^{-13} \\
& & 1.4 \text{ K} \leq \theta \leq 4 \text{ K} \ (\text{Bi}), & & &
\end{align*}\]

with $U_E$ in centimeters per second and $\theta$ in Kelvin degrees.

The equation (1) represents the balance of energy and (2) is a generalization of the Maxwell–Cattaneo equation. In fact, if $\alpha$ is a constant, (2) becomes

$$\tau \partial_i q + \kappa \text{grad} \theta = -q,$$  \hspace{1cm} (5)

i.e., the Cattaneo equation ($\tau = \kappa \alpha/\nu'$ is the relaxation time), while the classical Fourier law is obtained when $\alpha = 0$. A detailed discussion of the previous system is performed in [2]. We briefly observe that the system (1)–(2) is a particular case of a quasi-linear first-order system

$$A^o(u) \partial_i u + A^i(u) \partial_i u = f(u) \quad (i = 1, 2, 3),$$  \hspace{1cm} (6)

where $A^o$ and $A^i_n = A^i n_i$ ($n \in \mathbb{R}^3$ is the unit vector normal to the wave front) are $(4 \times 4)$ matrices and $f(u) \in \mathbb{R}^4$ is the source vector. In fact, by the identification

$$A^o = \begin{pmatrix} \rho c_v & 0 \\ \alpha' q & \alpha I \end{pmatrix}, \quad A^i_n = \begin{pmatrix} 0 & n \\ \nu' n & 0 \end{pmatrix}, \quad f(u) = \begin{pmatrix} 0 \\ \nu'/\kappa q \end{pmatrix},$$

the system (6) reduces to (1)–(2).
The characteristic velocities $\lambda \equiv \lambda(u, n)$ associated to (6) are the roots of the characteristic polynomial
\[ \det(A_n - \lambda A^\nu) = 0. \] (8)
It follows, in the present case, that the characteristic velocities are $\lambda = 0$, with multiplicity 2, and the roots of
\[ \rho c_o \alpha \lambda^2 + \lambda \alpha' q_n - \nu' = 0, \] (9)
where $q_n = q \cdot n$.

3. DISCONTINUITY WAVES

Recall at first, very briefly, the general outlines of the discontinuity wave theory. For a normalized hyperbolic first-order quasi-linear system in one-dimensional space
\[ \partial_t u + A(u) \partial_x u = f(u), \] (10)
it is possible to consider a particular class of solutions characterizing the so-called weak discontinuity waves.

In particular, the fields $u_o$ (unperturbed field) and $u$ (perturbed field) have, across the wave front $\Sigma$, a discontinuous normal derivative, i.e.,
\[ [u] = 0, \quad \delta u = [\partial u / \partial \varphi] = \Pi \neq 0, \] (11)
the square brackets representing the jump of any quantity evaluated on $\Sigma$ of cartesian equation $\varphi(x, t) = 0$. The jump vector $\Pi$ is proportional to the right eigenvector $d$ of the matrix $A$, evaluated in $u_o$; i.e., $\Pi = \Pi d(u_o)$, while the amplitude $\Pi$ satisfies a Bernoulli equation
\[ \frac{d\Pi}{dt} + a(t)\Pi^2 + b(t)\Pi = 0. \] (12)
In the case of a one-dimensional system [20–22] one has $d/dt = \partial_t + \lambda_o \partial_x$ indicating the time derivative along the characteristic lines $dx/dt = \lambda_o$ and $a(t), b(t)$ are known functions of time through $u_o$.

\[ a(t) = \varphi_x(\nabla \lambda \cdot d)_o, \] (13)
\[ b(t) = \left\{ d^T((\nabla l)^T - \nabla l) \cdot \frac{d u}{dt} + (\nabla \lambda \cdot d)(1 \cdot u_x) - \nabla (1 \cdot f) \cdot d \right\}_o, \] (14)
\[ \frac{d \varphi_x}{dt} + (\nabla \lambda \cdot u_x)_o \varphi_x = 0, \quad \varphi_x(0) = 1. \] (15)
Here $\nabla \equiv \partial / \partial u$, the index represents the derivative with respect to $x$, $\mathbf{l}$ is the left eigenvector of $A$ and, owing to the hyperbolicity, it is possible to choose it such that $l^{(i)} \cdot d^{(j)} = \delta^{ij}$; the index $o$ denotes the quantities evaluated in the unperturbed field $u_o$. The solution of (12) is

$$\Pi(t) = \frac{\Pi(0) e^{-\int_{o}^{t} b(\xi) d\xi}}{1 + \Pi(0) \int_{o}^{t} a(\xi) e^{-\int_{o}^{\xi} b(\eta) d\eta} d\xi}.$$  \hspace{1cm} (16)

If the wave satisfies the genuine non-linearity condition $\nabla \lambda \cdot d \neq 0$ there exists, for a suitable initial amplitude $\Pi(0)$, a critical time such that the denominator of (16) tends to zero and the discontinuity becomes unbounded. This instant corresponds, usually, to the formation of a strong discontinuity (shock wave) and so the field itself presents a discontinuity across the wave front [22, 23]. In the case of a constant equilibrium state $u_o$ the discontinuity wave amplitude $\Pi$ given by (16) becomes

$$\Pi(t) = \frac{\Pi(0) e^{-bt}}{1 - (a/b) \Pi(0) (e^{-bt} - 1)}.$$  \hspace{1cm} (17)

By imposing that the denominator of (17) vanishes, the critical time follows

$$t_{cr} = -\frac{1}{b} \log \left[ 1 - \frac{\Pi_{cr}}{\Pi(0)} \right],$$  \hspace{1cm} (18)

where we define

$$\Pi_{cr} = -\frac{b}{a}$$  \hspace{1cm} (19)

representing the threshold amplitude such that if $|\Pi(0)|$ is greater than $|\Pi_{cr}|$ a shock arises. In fact, from (18), to have $t_{cr}$ positive, by taking into account that $b > 0$ because the system (1)-(2) is supposed to be dissipative, the following conditions must be verified

if $a > 0 \rightarrow \Pi(0) < \Pi_{cr} = -\frac{b}{a} < 0$,  \hspace{1cm} (20)

if $a < 0 \rightarrow \Pi(0) > \Pi_{cr} = -\frac{b}{a} > 0$.  \hspace{1cm} (21)

As we prove later, in the present case, the coefficient $a(t)$ can change its sign owing to the loss of a genuine non-linearity condition and this implies that two different regimes for the discontinuity wave propagation may take place.
4. THE COEFFICIENTS OF THE TRANSPORT EQUATION AND THE CRITICAL TIME

To examine the problem of discontinuity waves associated to the system (1)–(2) let us consider the unidimensional case and assume, as unperturbed field, \( u_o = (\theta_o, q_o) \) with \( \theta_o = \text{constant}, q_o = 0 \) (equilibrium state).

First of all, we evaluate the coefficients of the transport equation (12). Since

\[
(\delta \lambda)_o = (\nabla \lambda \cdot \delta u)_o = \Pi (\nabla \lambda \cdot d)_o, \tag{22}
\]

we obtain, in the present case, taking also into account the calculations performed in [2]:

\[
(\delta \lambda)_o = \frac{3}{2} \left( \frac{U_E}{\Phi} \frac{d\Phi}{d\theta} \right) d\theta \quad \Phi(\theta) = U_E(\theta) \theta^{5/6}. \tag{23}
\]

Then, from (13), (15), and (22) the coefficient \( a \) is easily found

\[
a = \frac{5}{4} \frac{U_E}{\theta} + \frac{3}{2} U'_E = \frac{5A + B\theta^n(5 - 3n)}{4\theta(A + B\theta^n)^{3/2}}. \tag{24}
\]

This coefficient vanishes when

\[
\theta = \tilde{\theta}, \quad \text{with} \quad \tilde{\theta} = \left[ \frac{5A}{B(3n - 5)} \right]^{1/n}, \tag{25}
\]

where \( \tilde{\theta} (\tilde{\theta} = 3.38 \text{ K for Bi and } \tilde{\theta} = 15.36 \text{ K for NaF}) \) is the characteristic temperature pointed out formerly in [1–3]. In the present case too, this temperature plays an important role: in fact, in the next section, we show that when \( \theta \) “cross through” the critical temperature \( \tilde{\theta} \) the genuine non-linearity is lost and so the coefficient \( a(t) \) changes its sign (see (13)) determining two different regimes for the wave propagation.

The evaluation of the coefficient \( b \) requires to know the left eigenvector \( \mathbf{l} \) of the matrix \( A \). The left eigenvector \( \mathbf{l}^* \) of the non-normalized system is

\[
\mathbf{l}^*(A^o - \lambda A^o) = 0, \tag{26}
\]

and we find, for \( \lambda \neq 0 \),

\[
\mathbf{l}^* = \begin{pmatrix} 1 \\ 1 \\ \lambda \alpha \end{pmatrix}. \tag{27}
\]
Then, since the normal left eigenvector is related to $I^*$ by

$$ \mathbf{l} = I^* \mathbf{A}^\circ, $$

(28)

it follows, remembering (7),

$$ \mathbf{l} = \left( \rho c_v + \frac{\alpha' q}{\lambda \alpha}, \frac{1}{\lambda} \right). $$

(29)

The normalization factor $\beta$ of the right eigenvector (see [2]),

$$ \mathbf{d} = \beta \left( \frac{1}{\rho \lambda c_v} \right) $$

(30)

is evaluated by exploiting the formula

$$ \mathbf{l} \cdot \beta \mathbf{d} = 1, $$

(31)

and one gets

$$ \beta = \frac{1}{2 \rho c_v + (\alpha' q / \alpha \lambda)}. $$

(32)

At the equilibrium state ($q = 0$), (32) reduces to

$$ \beta_o = \frac{1}{2 \rho c_v}. $$

(33)

The term $\alpha'/\alpha$ can be calculated by taking into account (3)2, yielding

$$ \frac{\alpha}{\alpha'} = - \frac{U_E(\theta) \sqrt{c_v(\theta)} + \theta U'_E(\theta) \sqrt{c_v(\theta)} + \theta U_E(\theta) \left( c'_v(\theta) / 2 \sqrt{c_v(\theta)} \right)}{\theta U_E(\theta) \sqrt{c_v(\theta)}}. $$

(34)

From (14), for $u_o = \text{constant},$

$$ b = - \nabla (\mathbf{l} \cdot \mathbf{f})_o \cdot \mathbf{d}_o. $$

(35)

Recalling that $\nu'/\alpha = U_E^2 \rho c_v$ (see [2]), we easily obtain

$$ \mathbf{l} \cdot \mathbf{f} = - \frac{q \rho c_v}{\lambda \kappa} U_E^2, $$

(36)
and so, from (35),

\[ b = \frac{\rho c_p}{2 \kappa} U_E^2, \]  

(37)

that results always positive, as already observed.

At this point it is a simple matter to write

\[ \Pi_{cr} = -\frac{b}{a} = -2 \frac{\rho \varepsilon}{\kappa} \theta^4 \frac{\sqrt{A + B\theta^n}}{5A + B\theta^n(5 - 3n)}, \]  

(38)

or, substituting (25) in (38) and remembering (4),

\[ \Pi_{cr} = -\frac{1}{BDU_E} \frac{2\theta}{(3n - 5)(\tilde{\theta}^n - \theta^n)}, \]  

(39)

with the thermal diffusivity, a reliable indicator of the thermal properties of the material, given by

\[ D = \frac{\kappa}{\rho c_p} = \frac{\kappa}{\rho \varepsilon \theta^3}. \]  

(40)

With the previous choice of the right eigenvector, by taking into account (11) and the condition \( \Pi = \Pi d(u_o) \), the amplitude \( \Pi \) can be represented as

\[ \Pi(t) = -\frac{\lbrack \theta_r \rbrack}{U_E} = \frac{\lbrack \theta_x \rbrack}{U_E}. \]  

(41)

Hence, by means of the last formula and recalling (37) and (39), the amplitude (17) can be rewritten as

\[ \lbrack \theta_x \rbrack(t) = \frac{\lbrack \theta_r \rbrack(0) e^{-(U_E^2 / 2D)t}}{1 - \left[ BD(3n - 5)(\tilde{\theta}^n - \theta^n) U_E \lbrack \theta_x \rbrack(0) / 2\theta \right] \left( e^{-(U_E^2 / 2D)t} - 1 \right)}. \]  

(42)

From (18) we also have, by remembering (37), the critical time

\[ t_{cr} = -\frac{2D}{U_E^2} \log \left[ 1 - \frac{\Pi_{cr}}{\lbrack \theta_r \rbrack(0)} \right]. \]  

(43)

When the heat conductivity \( \kappa \) is infinite, from (37) \( b = 0 \) is obtained and so (16) furnishes

\[ t_{cr} = -\frac{1}{a \lbrack \theta_x \rbrack(0)}. \]  

(44)
Then, to have a positive critical time, the following situations must hold

(i) if $\theta < \tilde{\theta}$ one has $a > 0$ and so $[\theta_x](0) < 0$,
(ii) if $\theta > \tilde{\theta}$ one has $a < 0$ and so $[\theta_x](0) > 0$.

5. NUMERICAL TESTS WITH FINITE THERMAL CONDUCTIVITY

If the heat conductivity $\kappa$ has a finite value, a numerical simulation must be accomplished. It should be underlined that, contrary to our previous papers [1–3], at present the behaviour of $\kappa$ as a function of $\theta$ in the wave propagation at low temperatures is taken into account (a numerical code for the integration of the system (1), (2) when $\kappa = \kappa(\theta)$ has been developed also in [15]).

In what follows, we present the results regarding NaF crystals where $\rho \varepsilon = 23$ erg cm$^{-3}$ K$^{-4}$ and $\kappa = \kappa(\theta)$ is experimentally known [18]. In particular, to perform the calculations we have chosen a curve fitting (regression) for $\kappa$ constituted by a sixth-order polynomial.

In Fig. 1 the graph of the threshold amplitude $\Pi_{cr}$ vs. the temperature $\theta$ is represented. Here the critical temperature $\hat{\theta}$ appears as a critical value determining two different regimes for the discontinuity wave propagation. In fact, it is clearly seen that, when $\theta < \hat{\theta}$, the threshold amplitude is negative and so, recalling (20), only discontinuity waves with a negative initial value of the amplitude $[\theta_x]$ smaller than $\Pi_{cr}$ can degenerate. On the contrary, when $\theta > \hat{\theta}$, the threshold amplitude is positive and, from (21), only discontinuity waves with a positive initial value $[\theta_x]$ greater than $\Pi_{cr}$ can degenerate. Finally, note that the absolute value of $\Pi_{cr}$ changes through $\hat{\theta}$ in such a way that it is more easy to “produce” a shock wave when $\theta < \hat{\theta}$ with respect to the case with $\hat{\theta} > \theta$, where only large initial discontinuities ($> 400$ K/cm) can degenerate. The critical times and the corresponding critical lengths, given by $x_{cr} = U_E \cdot t_{cr}$ (the wave front starts, when $t = 0$, at $x = 0$), can be computed as functions of $\theta$ for fixed initial amplitudes choosing, for example, $\theta > \hat{\theta}$ and $[\theta_x](0) > \Pi_{cr}$ as shown in Fig. 2. Here the critical times (Fig. 2) and lengths (Fig. 3) for different positive values of $[\theta_x](0)$ decrease when $[\theta_x](0)$ increases. It is interesting to note that these values are comparable with the physical dimension (about $< 1$ cm) of the crystals and so, producing suitable initial discontinuities, it should be possible to experimentally verify our model.

Finally, we present in Fig. 4 a general three-dimensional plot of the critical time as a function of $\theta$ and $[\theta_x](0)$, in the case $\theta > \hat{\theta}$ and $[\theta_x](0) > 0$. It summarizes and extends, in an obvious way, all our previous observations: in particular, the “lowland” region, at the left corner, imme-
FIG. 1. The threshold amplitude $\Pi_{cr}$ vs. the temperature for NaF. The critical temperature $\bar{\theta}$ ($\bar{\theta} = 15.36$ for NaF) determines two different regimes for the discontinuity wave propagation.

FIG. 2. The critical times vs. the temperature $\theta(>\bar{\theta})$, for different positive values of $[\theta_{x}]^{(0)}$. 
Critical Lengths for Different Initial Positive Discontinuities in NaF

FIG. 3. The critical lengths vs. the temperature $\theta(>\theta)$, for different positive values of $[\theta_2]_0$.

Critical Time as Function of Temperature and Initial Discontinuity

FIG. 4. Three-dimensional plot of the critical time as a function of $\theta$ and $[\theta_2]_0$. 
6. A REMARK

Until now, our study of a discontinuity wave has provided us with the evolution of a point of an initial pulse generated in the heating process and supposed that at least a point exists where the derivative of the temperature with respect to the $x$ direction is discontinuous. But, in our opinion, for a real heating process abrupt enough, there would be two discontinuity points for the derivative, as sketched in Fig. 5. Note that each of these discontinuity wave fronts propagates in a constant state, represented by the horizontal parts of the profile at the right of $x_1$ and $x_o$ (in this last case we suppose that the thermal processes are able to create a local constant state).
Using this point of view, it is possible to express the hypotheses about the evolution of the wave profile drawn in Fig. 5. In fact, recalling the conditions to have a finite critical time and considering that now, in a unique wave front, two discontinuities propagating in a constant state are present (one positive in $x_o$, one negative in $x_1$), two possible degenerations can arise, as sketched in Figs. 6 and 7. Obviously, such considerations are applicable in the case of a cold initial profile too (i.e., when $\theta_1 < \theta_o$).

Finally, to complete our arguments, we underline two things. The first one is that, contemporaneously with the growth of the discontinuities, there also is the progressive deformation of the continuous profile (see [3] in the case of infinite heat conductivity). However, some numerical checks clearly show that, except for extreme conditions, the critical time for a discontinuity is less than the one related to the continuous profile. So, what happens in an abrupt heating of a face of a crystal would have to be similar to the behaviours illustrated in Figs. 6 and 7.

The second thing is that there is a convergence between the present conclusions and those for the shock waves obtained in [2] (see, in particular, Figs. 2 and 4 in [2] corresponding to Figs. 6 and 7 here). Because the
shape changes are in a good agreement with the available experiments [2] we are once more supported by a different point of view about the validity of our starting model.

7. CONCLUSIONS

In this paper, we have studied the behaviour of discontinuity waves in a rigid heat conductor at low temperature by also taking into account the experimental data for the thermal conductivity. From a mathematical point of view it is worth underlining that the existence of two different regimes for the discontinuity wave propagation, when the temperature values "cross" $\tilde{\theta}$, arises because the coefficient $a$ of the Bernoulli's equation changes its sign since the genuine non-linearity condition, $\nabla \lambda \cdot \mathbf{d} \neq 0$, is lost when $\theta = \tilde{\theta}$.

From a physical point of view, we note that our numerical simulations and the interpretation of the shape changes of the initial profile are in a
good agreement with our previous results (see [1–3]) and could be useful to perform suitable experiments to check the validity of the theory.

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