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Technical Notes

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Thermal Choke of the Evaporation Wave During Laser Ablation

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Nomenclature

c_p = specific heat
h = specific enthalpy
h_{fg} = latent heat of evaporation
M = Mach number
p = pressure
q = heat addition
R = gas constant
s = entropy
T = temperature
v = velocity
z = compressibility factor
γ = ratio of specific heats
ρ = density

Subscripts

s = value at the stagnation point
0 = value for the excited solid phase
1 = value for the gaseous phase

Superscripts

$*$ = value at the sonic point

Introduction

LASER ablation has a wide range of applications in engineering and scientific research. The laser ablation process during short-pulsed laser operation consists of three coupled processes: 1) heat conduction within the solid, 2) flow through a discontinuity layer attached to the solid surface, and 3) shock wave expansion of the laser-induced vapor/plasma. Tremendous research efforts have been directed toward understanding of the laser ablation process. Krokhin [1] was the first to formulate the physical mechanism of evaporation coupled with expansion of vapor and plasma. He postulated that the vapor leaving the evaporation wave is of sonic speed. Anisimov [2] and Knight [3] independently proved that the velocity of the vapor leaving the evaporation wave cannot exceed the speed of sound. Von Allmen [4] summarized the governing equations for the evaporation wave and presented two formulations. In the first formulation, the conservation equations together with the state equation form a well-posed problem. In the second formulation, the conservation equations together with the speed of sound form a well-posed problem. No attempt has been made to reconcile the ambiguity. Kelly and Braren [5] investigated the effects of the Knudsen layer on laser ablation. They suggested that the flow leaving the evaporation wave is approximately of sonic speed.

The previous studies either concluded or postulated that the velocity of vapor leaving the evaporation wave is limited by the speed of sound. However, the mechanism of the evolution of the evaporation wave during laser ablation remains unclear. In the present Note, the flow through the discontinuity layer attached to the solid surface is studied based on a compressible flow framework. The evaporation wave behaviors under different conditions are discussed.

The formulation of the physical mechanism of evaporation coupled with vapor expansion follows that of Krokhin [1]. During the laser ablation of materials, the laser energy is absorbed within a short penetration depth of the material. This leads to an increase of the surface temperature. A transient one-dimensional model can be used to describe the heat diffusion process within the solid. When the temperature of the material becomes sufficiently high, evaporation of the material occurs. At high laser intensity, the surface temperature is superheated to a temperature far beyond the saturation temperature to support the finite rate of evaporation. At this stage, the thermal diffusion stops playing a significant role. Without loss of generality, single-step evaporation from solid to vapor is assumed. The high-temperature solid expands into a rarefaction wave and experiences a phase change to vapor. The schematic of the evaporation wave is shown in Fig. 1. The solid surface recedes at velocity v_0 during laser ablation. The evaporation wave appears to be unsteady. A coordinate transformation can be done by attaching the moving evaporation wave to the receding solid surface. This simplifies the conservation equations across the evaporation wave, which can be expressed as

$$\rho_0 v_0 = \rho_1 v_1 \tag{1}$$

$$p_0 + \rho_0 v_0 v_0 = p_1 + \rho_0 v_0 v_1 \tag{2}$$

$$h_0 + \frac{v_0^2}{2} = h_1 + \frac{v_1^2}{2} \tag{3}$$

where ρ is the density, v is the velocity, p is the pressure, and h is the specific enthalpy. The subscript 0 indicates values for the superheated solid phase, and the subscript 1 indicates values for the gaseous phase. Because of the large difference between the density of solid and vapor, the velocity of vapor is much larger than the velocity of solid ($v_1 \gg v_0$). The $v_1 + v_0$ on the right-hand side of the conservation equations is reduced to v_1. This simplification has been commonly used by previous researchers [1]. The vapor generated then expands into a shock wave. The expansion process of the laser-induced vapor/plasma can be expressed by Euler equations. A detailed formulation of the laser ablation can also be found in Zhang et al. [6].

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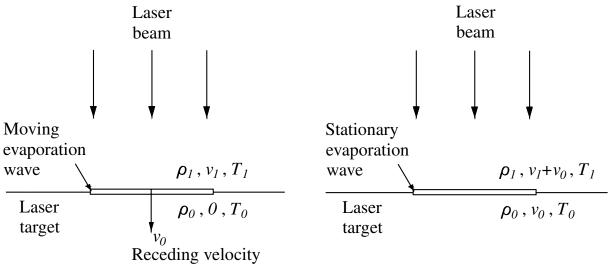

a) Evaporation wave in the reference frame of the laboratory **b) Evaporation wave in the reference frame attached to the receding surface**

Fig. 1 Schematic of the evaporation wave.

The evaporation wave is a finite rarefaction wave in nature, in which the pressure and density decrease as the velocity increases. It is well known that a finite adiabatic rarefaction wave experiences a decrease in entropy and thus is impossible to occur. This dictates that the evaporation wave be a finite rarefaction wave subject to heat addition, which is due to the difference between specific heats of solid and vapor and the latent heat of evaporation. The enthalpies of the solid and vapor can be expressed as

$$h_0 = c_{p,0}T_0 \tag{4}$$

$$h_1 = c_{p,0}T_{\text{sat}} + h_{\text{fg}} + c_{p,1}(T_1 - T_{\text{sat}}) \tag{5}$$

where T is the temperature, T_{sat} is the saturation temperature, h_{fg} is the latent heat of evaporation, and $c_{p,0}$ and $c_{p,1}$ are the specific heats of solid and vapor, respectively. The enthalpy of the solid can be split into two terms: $c_{p,1}T_0 + (c_{p,0} - c_{p,1})T_0$. The first term is the enthalpy of vapor evaluated at the solid temperature. The second term is the enthalpy difference between solid and vapor due to different specific heats of solid and vapor. The conservation of energy equation becomes

$$c_{p,1}T_0 + (c_{p,0} - c_{p,1})T_0 + \frac{v_0^2}{2} = c_{p,0}T_{\text{sat}} + h_{\text{fg}} + c_{p,1}(T_1 - T_{\text{sat}}) + \frac{v_1^2}{2} \tag{6}$$

This equation can be simplified to

$$h'_0 + q + \frac{v_0^2}{2} = h'_1 + \frac{v_1^2}{2} \tag{7}$$

$$q = (c_{p,0} - c_{p,1})(T_0 - T_{\text{sat}}) - h_{\text{fg}} \tag{8}$$

$$h'_0 = c_{p,1}T_0 \tag{9}$$

$$h'_1 = c_{p,1}T_1 \tag{10}$$

where q is heat addition, h'_0 is the enthalpy of vapor evaluated at temperature T_0, and h'_1 is the enthalpy of vapor at temperature T_1. It can be seen that rearranging the conservation of energy equation leads to an extra term q, which is due to the difference between specific heats of solid and vapor. According to Dulong–Petit law, the specific heat of solid is greater than that of vapor, generally. Additionally, at high laser intensity, the surface temperature is superheated to a temperature far beyond the saturation temperature. Therefore, q is always positive during the laser ablation. This shows that the evaporation process can be treated as flow with heat addition, which is caused by the difference between specific heats of solid and vapor. Once this treatment is established, classic analysis of thermal choke behavior of compressible gases can be applied to the evaporation wave during laser ablation. This type of treatment has been applied to other physical processes, such as the evaporation or condensation of liquid droplet in a gas stream. For example, Guha [7] developed a theory of thermal choke due to nonequilibrium condensation. He treated the condensation process as flow with heat interaction and derived an expression for the critical heat addition due to condensation.

The conservation equations for the evaporation wave [Eqs. (1–3)] can be written in differential forms as

$$\frac{d\rho}{\rho} + \frac{dv}{v} = 0 \tag{11}$$

$$dp + \rho v\, dv = 0 \tag{12}$$

$$dh + v\, dv = \delta q \tag{13}$$

The conservation of energy equation can be rearranged and expressed by

$$\frac{\delta q}{dv} = \frac{dh + v\, dv}{dv} = c_{p,1}\frac{dT}{dv} + v \tag{14}$$

The high-temperature solid and vapor obey the phenomenological state equation in the form of

$$p = z\rho RT \tag{15}$$

where z is the compressibility factor, and R is the gas constant. The state equation can be expressed in a differential form:

$$\frac{dp}{p} = \frac{dp}{z\rho RT} = \frac{d\rho}{\rho} + \frac{dT}{T} + \frac{dz}{z} \tag{16}$$

Substituting the conservation of mass and momentum into the state equation yields

$$-\frac{v\, dv}{zRT} = -\frac{dv}{v} + \frac{dT}{T} + \frac{dz}{z} \tag{17}$$

Rearranging the equation yields

$$\frac{dT}{dv} = \frac{T}{v} - \frac{v}{zR} - \frac{T\, dz}{z\, dv} \tag{18}$$

Substituting this equation into Eq. (11) gives

$$\frac{\delta q}{dv} = c_{p,1}\left(\frac{T}{v} - \frac{v}{zR} - \frac{Tdz}{zdv}\right) + v \tag{19}$$

$$= c_{p,1}\frac{T}{v} - \left(\frac{c_{p,1}}{zR} - 1 + \frac{c_{p,1}\rho T}{z}\frac{dz}{dp}\right)v \tag{20}$$

If the compressibility factor is constant at extremely high temperature and pressure, the equation is simplified to

$$\frac{\delta q}{dv} = c_{p,1}\frac{T}{v} - \left(\frac{c_{p,1}}{zR} - 1\right)v \tag{21}$$

Equation (18) shows that the flow is accelerated by heat addition when the flow velocity is small. When the flow velocity is sufficiently large, heat addition decelerates the flow. The transition point occurs when $\delta q/dv$ becomes 0. At this point, we have

$$c_{p,1}\frac{T}{v} = \left(\frac{c_{p,1}}{zR} - 1\right)v \tag{22}$$

That is,

$$v = \sqrt{\gamma zRT} \tag{23}$$

where γ is the ratio of specific heats, and $\sqrt{\gamma zRT}$ is the speed of sound for a compressible substance with a compressibility factor of z. Clearly, heat addition to the vapor flow at subsonic velocity results in an increase in the Mach number, whereas heat addition to the vapor flow at supersonic velocity decreases the Mach number. The limiting Mach number is unity. Because the maximum mass flux occurs at a Mach number of one, the evaporation wave is choked.

Realistically, the compressibility factor varies with pressure and temperature. For a variable compressibility factor, the transient point occurs at

$$c_{p,1}\frac{T}{v}=\left(\frac{c_{p,1}}{zR}-1+\frac{c_{p,1}\rho T}{z}\frac{\mathrm{d}z}{\mathrm{d}p}\right)v \tag{24}$$

The transition velocity will be shifted away from the speed of sound. Nevertheless, there is a transition point at which the evaporation wave is choked. For the sake of simplicity, the following analysis will be presented based on constant compressibility factor.

The evaporation wave subject to heat addition can also be shown on a Rayleigh line. The entropy of the vapor can be expressed by

$$s-s^*=c_{p,1}\ln\frac{T}{T^*}-zR\ln\frac{p}{p^*} \tag{25}$$

where superscript * indicates values at the sonic speed. For compressible substance, the pressure ratio can be expressed in terms of the temperature ratio [8]:

$$\frac{p}{p^*}=\frac{1+\gamma}{2}\pm\frac{\sqrt{(1+\gamma)^2-4\gamma(T/T^*)}}{2} \tag{26}$$

The entropy of the vapor now becomes

$$s-s^*=c_{p,1}\ln\frac{T}{T^*}-zR\ln\left[\frac{1+\gamma}{2}\pm\frac{\sqrt{(1+\gamma)^2-4\gamma(T/T^*)}}{2}\right] \tag{27}$$

A typical Rayleigh curve on a T (enthalpy)-s diagram is shown in Fig. 2. There are two temperature (enthalpy) values on the Rayleigh line for each entropy value. The top part of the curve represents the subsonic flow, and the bottom part represents the supersonic flow.

Because heat within the solid is conducted with a characteristic velocity of the sonic speed, the receding velocity of the solid surface cannot exceed the sonic speed during laser ablation. When the solid surface is receding at a subsonic speed, the heat addition increases the entropy and accelerates the flow velocity of the vapor leaving the evaporation wave. The heat addition increases with T_0, which increases with the laser intensity. Therefore, as the laser intensity increases, the flow velocity of the vapor leaving the evaporation wave increases as well. Once the sonic point is reached, the entropy reaches a maximum and the flow is thermally choked. The flow velocity of the vapor leaving the evaporation wave cannot increase without a significant change in the upstream conditions. The maximum heat addition $q_{\max}$ that the evaporation wave can accept corresponds to the area under the Rayleigh line and can be expressed by [8]

$$q_{\max}=c_{p,1}\left\{\frac{(1+\gamma M^2)^2}{2(1+\gamma)M^2[1+(\gamma-1)M^2/2]}-1\right\}T_{0,s} \tag{28}$$

where M is the Mach number of the receding solid surface, and $T_{0,s}$ is the stagnation temperature of the solid and can be expressed by

$$T_{0,s}=T_0[1+(\gamma+1)M^2/2] \tag{29}$$

When laser intensity increases further, additional heat beyond $q_{\max}$ will be added to the evaporation wave. Because the current Rayleigh line cannot accept additional heat, the evaporation wave will be forced to shift to a different Rayleigh line, as shown in Fig. 2. The surface temperature will increase beyond the temperature that is dictated by the rate of evaporation. Increased surface temperature decreases the receding velocity of the solid surface and raises the speed of sound. Thus, it reduces the initial Mach number. Because of the higher Rayleigh line, the excess heat addition can be accepted by the evaporation wave. Therefore, below the thermal choke threshold, the surface temperature will rise approximately logarithmically with the laser intensity, and the recoil pressure will increase linearly with the laser intensity [9]. The rate of increase of the surface temperature and recoil pressure with the laser intensity will be higher to accept heat addition beyond $q_{\max}$. As mentioned earlier, after the vapor leaves the evaporation wave, it expands into a shock wave. Because the vapor leaving the evaporation wave has a higher temperature and pressure beyond the thermal choke threshold, this will result in stronger shock wave during laser ablation. According to laser ablation theory [10], ambient gas can be heated to an extremely high temperature by strong shock wave. The high-temperature ambient gas increases the degree of ionization and thus the absorption of the incident laser. Therefore, the thermal choke mechanism has significant effect on the laser ablation process.

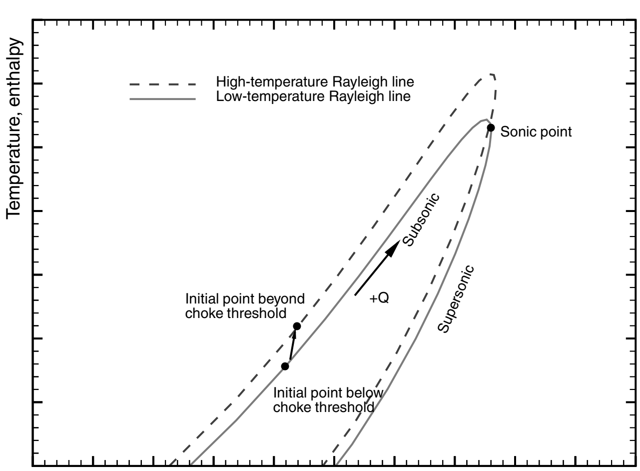

Fig. 2 Shift of the Rayleigh line by the evaporation wave.

Conclusions

This Note analyzes the thermal choke behavior of the evaporation wave during laser ablation. It was found that the discontinuity layer attached to the solid surface is a finite rarefaction wave subject to heat addition, which can be shown on a Rayleigh line. The heat addition is achieved due to different specific heats of the solid and vapor, and it increases the flow velocity for subsonic flow. As the laser intensity increases, the heat addition increases; the flow velocity of the vapor leaving the evaporation wave increases as well. Once the sonic point is reached, the flow is thermally choked. When laser intensity increases further and additional heat is added to the evaporation wave, the current Rayleigh line cannot accept any more heat, and the evaporation wave will be forced to shift to a different Rayleigh line. The evaporation wave will exhibit significantly different behavior beyond the thermal choke threshold.

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