# The Sublimation Energy of Metal versus Temperature and Pressure and its Influence on Blow-off Impulse

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*Abstract*—Based on the thermodynamic theory, the dependence of sublimation energy of metal on temperature and pressure is discussed, and the results indicate that the sublimation energy decreases linearly with the increase of temperature and pressure. Combined with this result, the blow-off impulse of aluminum induced by pulsed X-ray is simulated by smoothed particle hydrodynamics (SPH) method. The numerical results show that, while the change of sublimation energy with temperature and pressure is considered, the blow-off impulse of aluminum is larger than the case that the sublimation energy is assumed to be a constant.

*Keywords*—sublimation energy, blow-off impulse, pulsed X-ray, SPH method.

## I. Introduction

$\mathbf{W}$HEN the solid surface is radiated by the intense pulse (e.g., X-ray, electron beam or laser), part or all of the pulse energy is deposited in the surface and transmitted into the solid due to interaction between intense pulse and atoms of the solid. For the radiation time is very short (about ns level), a great deal of energy rapidly deposits in the material surface, and huge temperature and pressure grads are formed due to the fast attenuation of deposited energy from surface to inner, if the deposited energy is high enough to exceed the sublimation energy of the solid, the radiated solid surface will sublimate to gas immediately, then a blow-off impulse effect on the material takes place due to the forth ejection of gas. With these factors a shock wave, which is also called the thermal shock wave, is generated and travel through the target material. To simulate the blow-off impulse effect and thermal shock wave propagation, an equation of state which could describe both the expanding solid state and gas state is needed. In the codes of our program DRAM-08, the PUFF equation of state is adopted which has the

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general form as:

$$p = \rho \left[ G + \left( \Gamma_0 - G \right)(\frac{\rho}{\rho_0})^{1/2} \right] \left[ E - E_s \left\{ 1 - \exp[\frac{N\rho_0}{\rho}(1 - \frac{\rho_0}{\rho})] \right\} \right] \tag{1}$$

where $G = \bar{\gamma} - 1$, $N = c_0^2 / \left( \Gamma_0 E_s \right)$, $p$ is the pressure, $\rho$ is the density, $\rho_0$ is the normal density, $E$ is the specific internal energy, $E_s$ is the sublimation energy, $\Gamma_0$ is the normal Grüneisen coefficient, $c_0$ is the constant in the approximated linear relationship ($D = c_0 + su$) between the shock velocity ($D$) and particle velocity ($u$), and $\bar{\gamma}$ is the gas adiabatic exponent.

Research shows that the blow-off impulse and thermal shock wave propagation is close relative to the sublimation energy of material. To calculate the blow-off impulse correctly, the relation among the sublimation energy, the temperature and the pressure is deduced in this paper, and based on it, the blow-off impulse induced by the pulsed X-ray is calculated with the program DRAM-08 by using aluminum as the target material, last, the influence of changed sublimation energy on blow-off impulse is discussed detailedly, and some useful conclusions are obtained.

## II. Variation of Sublimation Energy with Temperature and Pressure

Based on the thermodynamics theory, for the first-order phase change at the temperature $T$ and pressure $P$, the latent heat of phase change can be described by Clapeyron equation as:

$$dp / dT = L / T (v_2 - v_1) \tag{2}$$

where $L$ is the latent heat of phase change, $v_1$ and $v_2$ are the specific volume before and after phase change respectively. For the phase change of sublimation, $v_1$ is the specific volume of solid and $v_2$ is the specific volume of gas. For the specific volume of gas state is much larger than that of solid state, the sublimation energy $E_s$ can be expressed as:

$$L = E_s = Tv\,dp/dT \tag{3}$$

where $v$ is the specific volume of gas state. Equation (3) indicates that the sublimation energy is relative to the

temperature and pressure. But by lack of vapor pressure data, it is very difficult to determine the exact change of sublimation energy with temperature and pressure from (3), then the thermodynamic theory is introduced to solve this difficult problem.

The basic thermodynamics differential equation for enthalpy $H$ (for 1 mol material) is:

$$dH = TdS + vdp \tag{4}$$

When $TdS = C_p dT - T \left( \partial v / \partial T \right)_p dp$ is substituted into (4), Equation (3) can be rewritten as:

$$\begin{aligned} dH &= C_p dT + [v - T(\partial v / \partial T)_p]dp \\ &= C_p dT + v(1 - \alpha T)dp \end{aligned} \tag{5}$$

where $H$ is the enthalpy, $\alpha$ is the coefficient of volume expansion, and $C_p$ is the specific heat at constant pressure. The enthalpy difference from one arbitrary state $x$ $(p_x, T_x)$ to the other state $y$ $(p_y, T_y)$ is:

$$H_y - H_x = \int_{T_x}^{T_y} C_p dT + \int_{p_x}^{p_y} v(1 - \alpha T)dp \tag{6}$$

Equation (6) is suitable for the sublimation of solid. Assume the pressure and temperature of initial state 1 is $p_1=0$, $T_1=0K$, and the final state 2 is $p_1=p$, $T_1=T$, which is the saturation state of solid (be sublimating), see Fig.1.

To calculate the enthalpy difference between state 1 and state 2, an integral is done along the reversible path from 1 to 2, where the most convenient path is along the isothermal path from 1 to A and then the isotonic path from A to 2. Thus the enthalpy difference between state 1 and state 2 is:

$$\begin{aligned} H_2 - H_1 &= \int_0^p v(1 - \alpha T)dp + \int_0^T C_{2p} dT \\ &= \int_0^p v dp + \int_0^T C_{2p} dT \end{aligned} \tag{7}$$

For the isothermal process from state 1 to state A, $\alpha = (\partial v / \partial T)_P / v = 0$. Eqution (7) reduces to:

$$H_2 = \int_0^T C_{2p} dT + \int_0^p v dp + H_1 \tag{8}$$

where $C_{2p}$ is the specific heat at constant pressure when pressure is $p$, and it can be taken as constant for its non-sensitivity to the pressure.

Then the enthalpy of saturation vapor is calculated. Assume that the saturation vapor is ideal gas, $C_P = (\partial H / \partial T)_P$, so the enthalpy is only a function of temperature:

$$H_3 = \int_0^T C_{3p} dT + H_{30} \tag{9}$$

where $H_{30}$ is the enthalpy of saturation vapor at 0K, and $C_{3p}$ is the specific heat at constant pressure.

If we assume that the sublimation of solid occurs at the state $(P, T)$, which is corresponding to the process from state 2 to state 3 in Fig.1. Then the sublimation energy is:

$$\begin{aligned} L = E_s &= H_3 - H_2 \\ &= \int_0^T C_{3p} dT - \int_0^T C_{2p} dT - \int_0^p v dp + H_{30} - H_1 \end{aligned} \tag{10}$$

This is the relation formula of sublimation energy with temperature and pressure, and the three integrals in the right-hand of (9) tend to be zero when the pressure and temperature are low enough. Then the sublimation energy $(E_{s0}=H_{30} - H_1)$ is just the sublimation energy at 0K, which can be obtained from some handbooks of material chemical and physical properties [1].
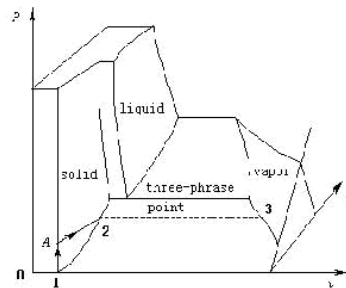


Fig. 1 $p$-$v$-$T$ curves of matter

For the static process, the vapor pressure is usually so low that the pressure integral in (10) can be ignored. Thus (10) can be rewritten as the Kirchhoff equation:

$$L = E_s = \int_0^T C_{3P} dT - \int_0^T C_{2P} dT + H_{30} - H_1 \tag{11}$$

Under the radiation of intense pulsed X-ray, the temperature and pressure of the material will increase rapidly with large energy absorbed by the surface layer within a very short time (ns level). When the energy absorbed is so high that has exceeded the sublimation energy of material, the solid surface will sublimate to gas, and the temperature and pressure increase quickly as well. For this case, the pressure integral in (10) can not be ignored, and the Kirchhoff equation is not appropriate any more.

Murnaghan equation is used to describe the relation between pressure and specific volume, and the pressure integral in (10) could be expressed as:

$$f \equiv \int_0^p v dp = \frac{An}{\rho_0 (n-1)} [(\frac{\rho}{\rho_0})^{n-1} - 1] \tag{12}$$

where A and n are the constants in Murnaghan equation.

The numerical analysis showes that the integral value $f$ and the pressure $p$ exhibit a good linear relation, which can be written as $p/\rho_a$, where $\rho_a$ is the average value of the density at the zero pressure and at the current pressure $p$. When (11) and (12) are applied to the monatomic molecule gas and the diatomic molecule gas, we can get some useful conclusions.

For the case that the sublimated gas is monatomic molecular gas, we get $C_{3p}=2.5R/M$, $C_{2p}=3R/M$, where $R$ is the universal gas constant and $M$ is the molecular weight of the metal. Consequently, the relation of sublimation energy with temperature and pressure follows the form:

$$E_s \approx E_{s0} - \frac{R}{2M}T - \frac{p}{\rho_a} \qquad (13)$$

For the case that the sublimated gas is the diatomic molecular gas, if the temperature is high enough, and the freedom degrees of molecular rotation and vibration are both excited [2], we have $C_{3p}=4.5R/M$, $C_{2p}=6R/M$. Then the sublimation energy can be written as:

$$E_s \approx E_{s0} - \frac{3R}{2M}T - \frac{p}{\rho_a} \qquad (14)$$

Equation (13) and (14) indicate that the sublimation energy is relevant to the temperature and pressure, and it decreases linearly with the increase of temperature and pressure.

## III. INFLUENCE OF THE CHANGE OF SUBLIMATION ENERGY ON BLOW-OFF IMPULSE

When the solid is radiated by intense pulsed X-ray, the blow-off phenomenon occurs in the solid surface and a thermal shock wave is formed. This process is simulated by SPH method, which is a pure Lagrangian particle method appropriate for large deformation problem and still being developed [3, 4]. We improve the SPH method based on [5] for its shortcoming in dealing with boundary problem [6]. In the SPH code the total blow-off impulse was expressed as [7]:

$$I = \sum_{u_j<0, E_j>E_s} m_j u_j \qquad (15)$$

where $m_j$ is the mass of particle $j$ which has sublimated, $E_j$ is the specific internal energy, and $u_j$ is the corresponding particle velocity.

During the numerical simulation, two blackbody spectra of 1 keV and 3 keV are considered respectively, the time spectrum is set as isoceles triangle with 40 ns bottom width, and the energy flux density $\Phi_0$ are 200 J/cm$^2$ and 300 J/cm$^2$. For the sublimation of aluminum materimal, when the surface of aluminum target is radiated by intense pulsed X-ray, it sublimates to gas immediately with large energy deposition. Gas

of aluminum is the monatomic molecular gas, so two cases are discussed respectively: the sublimation energy is assumed to be a constant (11.923 kJ/g), and the sublimation energy change with temperature and pressure according to (13).
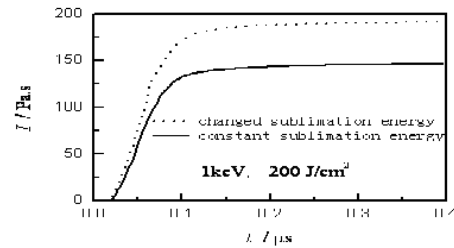


Fig. 2 The blow-off impulse induced by pulsed X-ray irradiating on aluminum,of which the energy spectrum is 1 keV blackbody spectrum, and the flux density is 200 J/cm$^2$


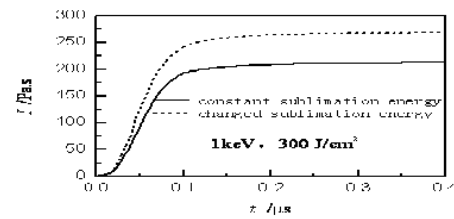
Fig. 3 The blow-off impulse induced by pulsed X-ray irradiating on aluminum,of which the energy spectrum is 1 keV blackbody spectrum, and the flux density is 300 J/cm$^2$
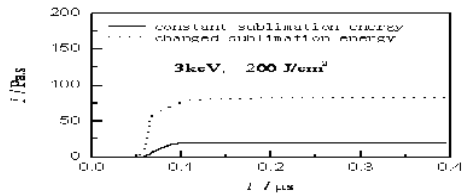


Fig. 4 The blow-off impulse induced by pulsed X-ray irradiating on aluminum,of which the energy spectrum is 3 keV blackbody spectrum, and the flux density is 200 J/cm$^2$
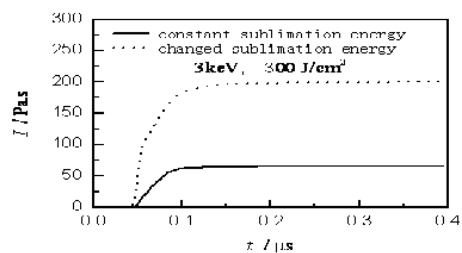


Fig. 5 The blow-off impulse induced by pulsed X-ray irradiating on aluminum,of which the energy spectrum is 3 keV blackbody spectrum, and the flux density is 300 J/cm$^2$

The numerical simulation results are shown in Fig.2- Fig.5. Fig.2 and fig.3 show the results of 1 keV (soft spectrum) blackbody spectrum, and fig. 4 and fig.5 show the results of 3 keV (hard spectrum) blackbody spectrum. In these figures, the solid line is corresponding to the blow-off impulse of aluminum

material while the sublimation energy is considered to be a constant, and the dashed line is corresponding to the blow-off impulse while the sublimation energy changes with temperature and pressure according to (13). It is obvious that the calculated blow-off impulse increased markedly when the sublimation energy varying with the temperature and pressure is considered, but the difference of blow-off impulse between the constant and changed sublimation energy cases tends to decrease when the energy fluence increases. The results also indicate that the harder the spectrum of X-ray is, the larger the difference of blow-off impulse between the two cases will be. So to calculate the blow-off impulse more accurately, the sublimation energy of target material changing with temperature and pressure must be considered.

## IV. CONCLUSION

The dependence of the sublimation energy on temperature and pressure is studied based on thermodynamics, and the blow-off impulse of aluminum induced by pulsed X-ray is simulated by SPH method in this paper. The conclusions we get are as follows:

(1) The sublimation energy decreases linearly with the increase of temperature and pressure.

(2) The influence of different sublimation energy values on blow-off impulse of aluminum induced by pulsed X-ray is significant. Compared to the case that the sublimation energy is assumsed to be a constant, if the variation of sublimation energy with temperature and pressure is considered, the calculated blow-off impulse is larger.

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