ANALYSIS OF DISSIPATIVE STRUCTURE IN MATERIAL COMMINUTION①

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ABSTRACT Dissipative structure formed in material comminution is pointed out. The behavior of thermodynamics and dynamics of material comminution is researched.

Key words: material comminution dissipative structure catastrophe nonlinear thermodynamics dynamics

1 INTRODUCTION

Over the past 100 years, the scholars of different countries were engaged in a great quantity of investigation work on energy consumption in comminution process. Some crushing theories such as Rittinger's law, Kick's law, Bond theory and others were proposed to uncover the relation and effect of energy consumption in comminution process. Such works were confined to the field of dynamics, equilibrium and continuous steady process. They did not mirror the outstanding characteristics of irreversibility, noncontinuity, catastrophe, nonlinearity and open system. For this reason, the author applied first catastrophe theory and dissipative structure to research the process of material comminution in the Ref. [1].

2 THE DISSIPATIVE STRUCTURE FORMED IN THE MATERIAL COMMINUTION

The reduction of material to a smaller size is known as comminution. Traditional research on mechanism of material comminution regarded comminution process as black box. It paid attention to the dynamic relation of input and output. Our research emphasizes the variation and process considering the following reasons:

(1) The material system is consisted of a host of particles(subsystems). Such system is just the object of study of thermodynamics.

(2) The temperature rising in the split will be happened suddenly when material is comminuted, for example, that of the quartz approaches to about 4 000 K.

(3) A small amount of the input energy in the process of material comminution (among others grinding occupies about 1%) is consumed to produce new surfaces. The rest is dissipated in the form of heat.

So the exploring on mechanism of comminution can not confine to the dynamics, and should open up the category including nonlinear dynamics and nonequilibrious nonlinear thermodynamics.

The comminution process is described by means of continuous functions in the traditional theory of comminution. To be sure, the comminution was considered as a successive change process, however quite the opposite, only when the outside force is big enough to overcome the cohesive force of the particles of material, can the comminution be happened suddenly. Therefore, the comminution of materials should be condisered as a catastrophic process.

One of the fundamental features of the

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catastrophic process is that the stability of the original state of system is lost and the system transits into a new state.

From the point of view of thermodynamics, the equilibrium state is always stable except phase change. So we can draw a conclusion that the unstability of the system occurs only for nonequilibrium.

In fact, the material comminution is a monodirectional process that the big lumps of material are changed into the small lumps. So material comminution is an irreversible process. A fundamental feature of the irreversible process is that the system is in the nonequilibrium of thermodyanmics as a result of existing energy dissipation inside the system. This is a necessary condition of the unstability of material system.

The system is in thermodynamic linear nonequilibrious stable state when the system deviates not far from equilibrium.

Deviating far from equilibrium is a necessary condition but not sufficient condition that the sytstem is unstable.

From the point of view of mathematics, a special state of the system correspounds to a special solution of the dynamic equation (the ordinary differential equation or the partial differential equation) describing the dynamic behavior of the system. So the unstable state correspounds with the unstable special solution of the differential equation. However, the order state of the system is described by stable special solution. So the dynamic equations that can correctly describe the dynamic behavior of the system must exist unstable and stable special solution. Such differential equations are inevitably nonlinear. Hence the dynamic process of the system certainly includes the proper nonlinear feedback. The comminution process of material is just so. The experiments on press crushing single particle and material layer indicate that the pressure versus deformation is nonlinear.

The order microstructure is formed and maintained by energy dissipation and nonlinear dynamic mechanism in course of exchanging substance and energy with outside in the condition of opening and deviating far from equilibrium. Prigogine called this structure after dissipative structure. As mentioned above, material comminution is an open system, material system is consist of a large number of material particles. The system is nonlinear and far from equilibrium, fluctuation in the system will not attenuate but will amplify. There occurs the catastrophe of the state of material system, the disorder state transforms into order one and thus the dissipative structure is formed. So we can expound the physical nature destroying old structure and forming new one in the process of material comminution with the thermodynamics of nonlinear irreversible process, and can expound the unstability and stability in the process of material comminution with the detail behavior of dynamics.

3 NONLINEAR THERMODYNAMICS AND DYNAMICS IN MATERIAL COMMINUTION

3.1 *Entropy Production, Extra Entropy and Extra Entropy Production*

Material comminution is an open system. Its entropy change is expressed as follows:

$$\begin{aligned} dS &= d_iS + d_eS \\ &= d_iS + \frac{\delta Q}{T} + [(S_{in}dm) \\ &\quad - (S_{out}dm)] \end{aligned} \tag{1}$$

where d_iS is the entropy production due to the irreversible process in the system; d_eS is the entropy flux including the effect of heat exchange $\delta Q/T$ and the effect of mass exchange $[(S_{in}dm) - (S_{out}dm)]$; dm is the mass change; S_{in} and S_{out} is respectively the specific entropy of inflow mass and outflow one.

The first term and the third term are positive in the Eq. (1), and the second term $\delta Q/T$ is negative when the system is exothermic. Only when $dS < 0$ can the material be comminuted.

The change rate of entropy production with time is called the rate of entropy production, for short it is called the entropy production:

$$P = \frac{d_i S}{dt} = \int_V \sigma dV = \int_V dV[\Sigma JX] \quad (2)$$

where σ is the entropy production of unit volume; J is the generalized flux; X is the generalized force.

The rate of variation of entropy production can be separated into two terms

$$\frac{dP}{dt} = \int dV[\sum_k J_k \frac{dX_k}{dt}] + \int dV[\sum_k X_k \frac{dJ_k}{dt}] = \frac{d_X P}{dt} + \frac{d_J P}{dt} \quad (3)$$

where $d_X P/dt$ represents the rate of variation of entropy production due to the change of forces, and $d_J P/dt$ results from the change of fluxes.

According to Onsager reciprocal relations and minimum entropy production principle in the linear region of nonequilibrium we obtain

$$d_X P = d_J P = \frac{1}{2} dP \leqslant 0 \quad (4)$$

In the nonlinear region of nonequilibrium if the boundary conditions are unconcerned with time, we can prove it with the assumption of local equilibrium that:

$$\frac{d_X P}{dt} \leqslant 0 \quad (5)$$

Due to the generality of the statement expressed by Eq. (5), it is called the universal criterion of evolution.

Being corresponded to Eq. (2) that the entropy production is defined as the product of force and flux, the extra entropy production is defined as

$$\delta_X P = \int dV[\sum_k \delta J_k \delta X_k] \quad (6)$$

where δX_k is extra force and δJ_k is extra flux.

For founding the relationship between entropy S and extra entropy production $\delta_x P$, S and P are expanded into Taylor series in the neighborhood of the steady state(S^0, P^0)

$$\left.\begin{aligned} S &= S^0 + \delta S + (1/2)\delta^2 S + \cdots \\ P &= P^0 + \delta P + (1/2)\delta^2 P + \cdots \end{aligned}\right\} \quad (7)$$

According to the assumption of local equilibrium, we obtain $\delta S = 0$, then:

$$(1/2)\delta^2 S = S - S^0 < 0 \quad (8)$$

In same time we have:

$$\frac{d}{dt}(\frac{1}{2}\delta^2 S) = \int dV[\sum_k \delta J_k \delta X_k] = \delta_X P \quad (9)$$

3.2 *Analysis of the State Stability of Material System*

State stability is such a problem of which the state can exist continuously and of that the unsteady state will change spontaneously.

For the equilibrium of thermodynamics, system stability can be determined by extreme value behavior of entropy S and its time evolution behavior dS/dt. In the linear region of nonequilibrium, $P > 0$ and $dP/dt \leqslant 0$ are the criterion of the system stability. That is, the entropy of equilibrium and the entropy production of linear region of nonequilibrium are the thermodynamic potential function that deseribes the stability of system state.

In the nonlinear region of nonequilibrium, entropy and entropy production are not the thermodynamic potential function. So, while thermodynamic method is applied, the stability of the system of nonlinear differential equations that describe nonlinear dynamic behavior is studied. If the solutions of the equations are steady, the system states are steady, too.

Because the great majority of the system of nonlinear differential equations (especially partial differential equations) can not obtain or very difficultly to solve analytic solutions, thus it is difficult to analyze the stability for the special dynamic equations, so we hope that the system stability can be judged under the circumstances not to solve the solutions of the equations. For this purpose we apply Lyapounov direct method of the stability theory of the system of the nonlinear differential equations.

An arbitrary higher order differential equation can be substituted by a group of the first oredr equations if each order derivative is considered as unknown.

$$\frac{dX_i}{dt} = f_i(X_1, X_2, \cdots, X_n)$$
$$(i = 1, 2, \cdots, n) \quad (10)$$

Assuming Eq. (10) to be existed zero solution and the function $V(X_1, X_2, \cdots, X_n)$ to exist continuous partial derivative for all X_i, then the function V has total derivative:

$$\frac{dV}{dt} = \sum_i \frac{\partial V}{\partial X_i} \frac{dX_i}{dt} = \sum_i \frac{\partial V}{\partial X_i} f_i(X_1, X_2, \cdots, X_n) \qquad (11)$$

Lyapounov's stability theory establishes the stability criterions of the solution of equation with the properties of function V and its total derivative:

when $V \frac{dV}{dt} \leqslant 0$, the zero solitions of Eq. (10) are steady;

when $V \frac{dV}{dt} < 0$, the zero solutions of Eq. (10) are asymptotic steady;

when $V \frac{dV}{dt} > 0$, the zero solutions of Eq. (10) are unsteady.

The function $V(X_1, X_2, \cdots, X_n)$ possessing such properties is called as Lyapounov function.

Applying the stability theory mentioned above, we can discuss the stability of non-zero steady state in Eq. (10)(even other special solutions) with the aid of the transformation of coordinates.

For the nonlinear system of nonequilibrium from Eq. (8), we obtain $(1/2)\delta^2 S \leqslant 0$ (it is equal to zero in the steady state). And that $\frac{d}{dt}(\frac{1}{2}\delta^2 S) = \delta_X P$ does not exist determinate positive sign or negative sign. Hence $(1/2)\delta^2 S$ is considered as Lyapounov function. The stability of reference state can be determined by the following creterions:

When $\frac{d}{dt}(\frac{1}{2}\delta^2 S) > 0$ (12a)

the reference state is asymptotic steady;

When $\frac{d}{dt}(\frac{1}{2}\delta^2 S) = 0$ (12b)

the reference state is critical steady;

When $\frac{d}{dt}(\frac{1}{2}\delta^2 S) < 0$ (12c)

the reference state is unsteady.

To sum up, there are the following features of thermodynamics and dynamics in the material comminution:

The first, material comminution is a process that the bigger lumps of material lose the stability and happen the suddenly catastrophe of changing into smaller lumps. This process satisfies the criterion condition of Eq. (12c). So material comminution is a process which changes the material from steady state to unsteady one, i. e. into new steady state.

The second, $(1/2)\delta^2 S = S - S^0 < 0$ must be satisfied when the material is comminuted, i. e., $dS < 0$ in Eq. (1). The first term and the third term in Eq. (1) are positive, and then in order to ensure $dS < 0$, material system must be exothermic, and the exothermic heat must satisfy

$$-\delta Q > T[d_i S + S_{in} dm - S_{out} dm] \qquad (13)$$

The equation above explains quantitatively the necessity that a small amount of input energy in the process of material comminution is consumed to form a new surface and a large number is dissipative in the form of heat, and the importance of thermodynamics to study the mechanism of comminution.

The third, when cracks extend fast, the temperature of split will be thousands degree Kelvin temperature, it reduces elastic modulus and strength of material and softens material and enhances the activation of crack extension. For this reason, decreasing heat exchange between equipment and environment should be considered in order to soften comminuted material with the heat produced in the process of comminution.

The fourth, from $\delta_X P < 0$, we know that $(1/2)\delta^2 S$ is decreasing progressively. When the assumption of local equilibrium is satisfied, entropy S is decreasing progressively, too. As viewed from economizing on energy in prerequisite to maintain the unsteady state of material system, the extra entropy should be strived to reduce, to cut down the dissipative velocity of energy.

4 CONCLUSION

(1) The research on mechanism of material comminution in this paper mirrors the outstanding features of irreversibility, noncontinuity, catastrophe, interference, nonlinearity deviating far from equilibrium in the process of

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(*From page 24*)material comminution.

(2) Proceed from catastrophe, irreversibility, state deviating far from equilibrium in the process of material comminution, the fundamental conditions forming dissipative structure are studied.

(3) Proceed from the unstability and stability of the state of material system, the mechanism research of material comminution is carried to the category of nolinear thermodynamics and nonlinear dynamics.

(4) System response to nonequilibrium constraints of outside is better described when extra entropy is regarded as the Lyapounov function of material system in order to judge the stability of the system.

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