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THEORETICAL CALCULATION AND SIMULATION ANALYSIS OF THE ENHANCED CRUSHING PROCESS OF HIGH NITROGEN STEEL MOLTEN DROPLET

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High nitrogen steel has been widely explored and developed due to their unique properties. At present, most of the references on high nitrogen steel powders prepared via gas atomization mainly focus on their initial and secondary crushing. The research on the enhanced crushing process caused by the "nitrogen escape" inside the high nitrogen molten steel is rare. In this paper, the enhanced crushing process of high nitrogen steel molten droplet is investigated based on the theoretical calculation and numerical simulation, which reveals the enhanced crushing mechanism of nitrogen-containing droplets in the process of preparing high nitrogen steel powders by atomization method.

Keywords: nitrogen steel, atomized molten droplets, enhanced crushing, theoretical calculation, numerical simulation

INTRODUCTION

The nitrogen element can improve the corrosion and wear resistance of high nitrogen steels [1,2]. Meanwhile, using the method of preparing of high nitrogen steel via gas atomization can effectively avoid nitrogen segregation and improve the sphericity of powder[3,4].

During the powder preparation process by gas atomization, high nitrogen steel firstly forms a liquid band of large size though initial crushing, and then the liquid band is disintegrated into a collection of atomized molten droplets, which will rapidly solidify into powder particles under the impact of high pressure and velocity gas stream during the process of secondary crushing [5,6]. At the same time, nitrogen bubbles may escape from the interior of some larger droplets, which will lead to the further crushing about the atomized molten droplets. This process will significantly affect the morphology, nitrogen content, and average particle size of the high nitrogen steel powders. Therefore, it is important to investigate the enhanced crushing mechanism, which plays the important role on tunable preparation of the high-quality powders.

THEORETICAL CALCULATION

Flow state analysis of atomized molten droplets

The schematic diagram of gas atomization process is depicted in Figure 1. It can be observed that the alloy melt flows down into the guide tube, while atomized gas is sprayed from the nozzle. Subsequently, the metal liquid stream enters a negative pressure zone from the liquid stream outlet, and then interacts with atomizing gas to accomplish the gas atomization process.

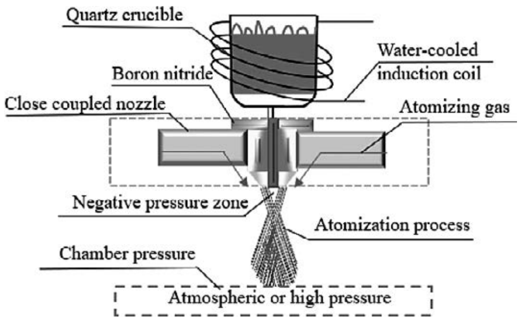

Figure 1 Schematic diagram of gas atomization process

As the enhanced crushing process occurs after the second atomization process, atomized molten droplets encapsulating nitrogen bubbles break away from the gas reflux zone, and then their trajectory will change under the airflow perturbation effect. Therefore, the flow state of atomized molten droplets can be determined by the formula of Reynolds number (*Re*) as follows:

$$\mathrm{Re} = \rho d V / \mu \tag{1}$$

Where ρ is the fluid density (kg/m^3), d is the feature length /m, V is the average velocity of the fluid (m/s), μ is the dynamic viscosity of the fluid (Pa/s), $Re<2\ 300$ for laminar flow and $Re>2\ 900$ for turbulent flow. When $\rho=7\ 431$ kg/m^3, $d = 10^{-4}$ m, $V=220$ m/s, $\mu=2\ 250$ Pa×s, the Re is calculated to be 0,072, which is less than 2 300, and further reveals that the flow state is laminar

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flow. Since the atomized molten droplets are in turbulent flow during the secondary atomization process, the atomized molten droplets can be supposed to the transition from turbulent flow to laminar flow in the enhanced crushing process, as observed in Figure 2.

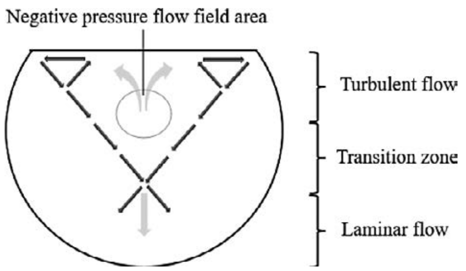


Figure 2 Schematic diagram of the nitrogen flow field

Enhanced crushing mode investigation

Under the condition of high chamber pressure, the interaction between the atomized molten droplet and high-speed nitrogen jet can be described to the interaction of gas breaking force, liquid viscosity force, and surface tension of atomized molten droplets, represented, which can be determined by formulas of Weber number (*We*) and Ohnesorge number (*Oh*) as follow [7,8]:

$$We = \frac{\rho_g U_r^2 d_0}{\sigma} \tag{2}$$

$$Oh = \frac{\mu_1}{\sqrt{\rho_1 d_0 \sigma}} \tag{3}$$

Where *We* and *Oh* are the ratio of gas dynamics to surface tension, and the ratio of liquid viscosity to surface tension, respectively. And d_0 is the atomized molten droplet diameter (m), ρ_g is the gas density (kg/m^3); *Ur* is the relative motion velocity between gas and liquid (m/s), σ is the atomized molten droplet surface tension (N/m), μ_1 is the atomized molten droplet viscosity (Pa/s), ρ_1 is the atomized molten droplet density (kg/m^3). When μ_1=2 500 Pa/s, ρ_g=7 431 kg/m^3, d_0 =10^{-4} m, and σ=1,5×10^6 N/m, *Oh* is calculated to be 2,131, which is greater than 0,1. Therefore, gas kinetic perturbation is the main reason of the enhanced crushing occurrence for atomized molten droplets.

According to *We* value, the crushing pattern of atomized molten droplets include the following modes as demonstrated in Table 1[9,10].

Table 1 **Selection of crushing models**

Crushing Mode	Range of *We*
Dumbbell Crushing	10,7 ≤ *We* ≤12
Bag Crushing	12 ≤ *We* ≤ 40
Multimode Crushing	40 ≤ *We* ≤ 100
Extended Crushing	100 ≤ *We* ≤ 350
Catastrophic Crushing	*We* ≥ 350

The *We* of the enhanced crushing process for secondary atomization process can be calculated with the help of further simplifying formulas:

$$We_p \approx \frac{18U_{r2}^2}{C_d U_{r1}^2} \tag{4}$$

$$C_d = \frac{10}{\sqrt{\mathrm{Re}}} \tag{5}$$

Where U_{r2} is the relative motion velocity between gas and liquid phases at the beginning of enhanced crushing (m/s), U_{r1} is the relative motion velocity between gas and liquid at the beginning of secondary atomization (m/s), C_d is the laminar flow shear stress constant. Through the above calculations, C_d and We_p can be determined to be 38,46 and 453,04.

Depending on the *We* determination in the Table 1, droplets are under the influence of gas kinetic perturbations, and their crushing mode is mainly catastrophic crushing. When atomized molten droplets burst into multiple small spherical droplets, irregular larger droplets may also appear, as presented in Figure 3.

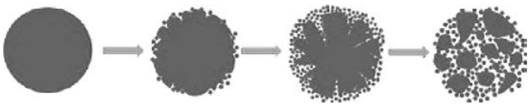


Figure 3 Catastrophic crushing diagram

When atomized molten droplets detach from the gas flow region, there is a sharp decrease in temperature. At the same time, turbulent eddy collisions can pressure increase outside. Subsequently, nitrogen bubbles split into two or more bubbles via shearing and shedding of the tail vortex. This dynamic process triggers the unstable changes between gas and liquid phases interface, and nitrogen bubble rupture will further prompt the enhanced crushing of the entire droplet, which is illustrated in Figure 4. From a balance perspective, the process of bubble rupture can be described as a balance between external breaking stress and internal surface tension within the bubble. The purpose of above behavior is to maintain the bubble shape.

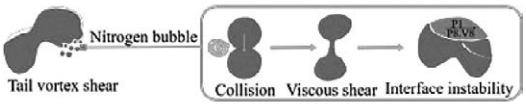


Figure 4 Schematic diagram of unstable changes between gas and liquid phases

According to stress analysis, the unstable changes of the gas and liquid phases in the atomized molten droplet can be attributed to the dumbbell crushing as depicted in Figure 5. In theory, this crushing mode will further refine the particle size of the powder and enhance its sphericity.

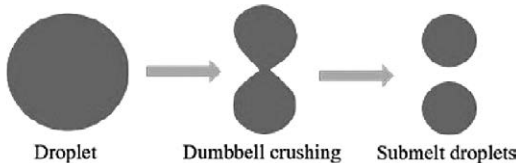
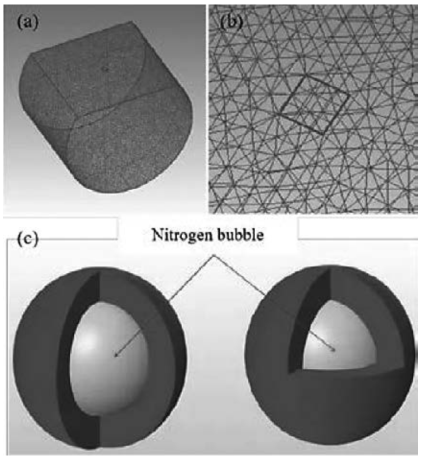


Figure 5 Schematic diagram of dumbbell crushing

SIMULATION ANALYSIS

The enhanced crushing process of high nitrogen steel molten droplets occur after the secondary atomization. For a better understanding of this process, using Ansys Fluent 16,0 to simulate the enhanced crushing process of droplets. The models are presented in Figure 6.



(a) Atomizer model; (b) Local features; (c) Atomized molten droplets

Figure 6 Schematic diagram of the relevant model structure

Analysis of post-processing for enhanced crushing process

After the global initialization, the volume fraction map of a single atomized molten droplet experiencing enhanced crushing is outputted and revealed in Figure 7. The central area is the nitrogen inside the droplet, surrounding area is the liquid high nitrogen steel. When enhanced crushing of a single droplet occurs, nitrogen bubbles expand, and the volume fraction is the highest. Meanwhile, the volume fraction of atomized molten droplet component is gradually decreases as the center moves away.

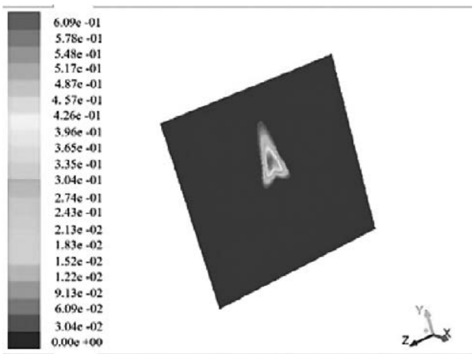


Figure 7 Cloud diagram of the volume fraction

To analyze the temperature change relationship between the liquid and gas phases of atomized molten droplets, adjusting the number of droplets to 10 and the chamber pressure to 0 MPa. After the numerical simulation, results are exported as shown in Figure 8. X-axis represents the isothermal gradient change of the atomized molten droplet liquid phase relative to the melting point temperature. Y-axis represents the numerical variation of gas phase temperature with liquid phase temperature.

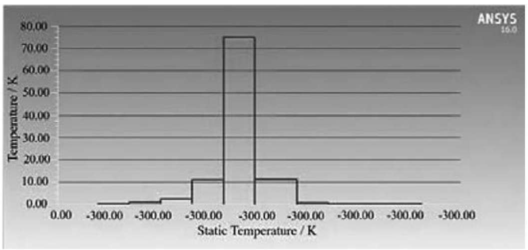


Figure 8 Numerical variation of gas phase temperature with liquid phase temperature

Based on the relationship analysis in Figure 8, the temperature change of gas phase with the variation of liquid phase can be calculated and obtained in Figure 9. It presents the effect of the temperature variation of the atomized molten droplet on enhanced crushing, which reveals that the liquid phase temperature drop range in the range of 600 to 900 K is the optimal temperature interval for the occurrence of enhanced crushing.

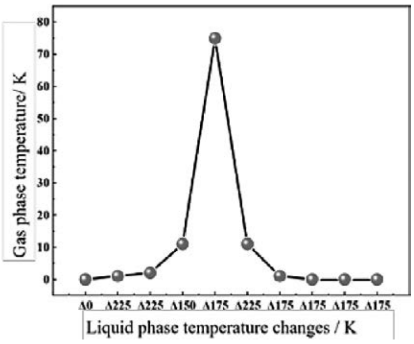


Figure 9 Temperature change of gas phase with the variation of liquid phase

After heat exchange, the expansion of the gas phase inside atomized molten droplets is higher than liquid phase. To investigate the mechanism of the nitrogen bubble pressure inside the atomized molten droplet on the liquid shell, the pressure variation of the internal gas phase is simulated and analyzed. As depicted in Figure 10, the gas phase pressure exhibits a gradient distribution. The optimum pressure value inside enhanced crushing is up to about 14 Pa, which is the most optimized criteria for the enhanced crushing process happening.

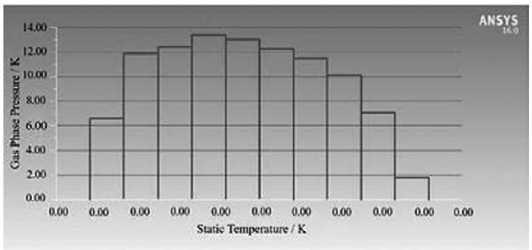


Figure 10 Distribution of gas phase pressure values

Analysis of factors affecting enhanced crushing

Investigating the density fluctuations of the molten droplet particle cluster is of crucial importance for analyzing the mechanism of enhanced crushing. The number of atomized molten droplets is adjusted to 1 000, and the atomizer chamber pressure is set to 0,3 MPa. Using the center of the atomizer model as the origin of the two-dimensional coordinate system, and the vertical downward direction along the Y-axis is used as the positive direction. When the material density is set to 7 431 kg/m^3, the density change curve can be obtained and shown in Figure 11. During the process from the secondary atomization to enhanced crushing, the liquid phase density of the atomized droplets along the Y-axis remain unchanged, indicating that the spherical shell of the atomized droplets is still in a liquid state.

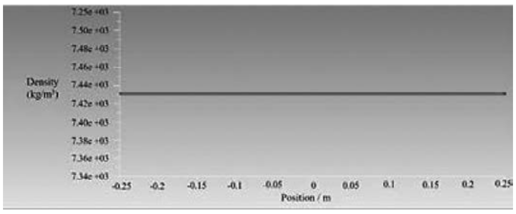


Figure 11 The density change curve about atomized molten droplet

In addition, the effect of its internal nitrogen density on enhanced crushing should also be considered. The nitrogen density at standard condition is 1,25 g/L, while at a critical temperature of -147°C and a critical pressure is 3,39 MPa, the corresponding nitrogen density is 0,81 g/L. The change in gas density under varying pressure and temperature is negligible. Through numerical simulation, it can be observed that the density of the droplet remains constant after leaving the gas reflux zone. Therefore, the density configuration in both gas and liquid phases of atomized molten droplets has no effect on the process of enhanced crushing.

CONCLUSION

Through above analysis, the conclusions are summarized as follows.

(1) Due to the instability of the gas and liquid phases interface, dumbbell crushing is an important form of enhanced crushing of atomized molten droplets.

(2) Within the atomized molten droplet, there is a heat exchange occurring between the gas and liquid phases. The decrease of liquid phase temperature will further lead to an increase in gas phase temperature.

(3) When the chamber pressure is 0 MPa, the gas phase pressure value on the atomized molten droplet can reach up to 14Pa, which is beneficial for the occurrence of enhanced crushing.

(4) At a chamber pressure of 0,3 MPa, the variations in liquid phase density and nitrogen density within the atomized molten droplet are not related to the enhanced crushing.

Acknowledgments

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Note: Responsible for English language is Q. Li.