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Research note

Growth characteristics of spherical titanium oxide nanoparticles during the rapid gaseous detonation reaction

Ning Luo[a,b,*], Hongwen Jing[a], Zhanguo Ma[a], Yingchao Wang[a], Guilei Sun[c], Weidong Liu[b]

[a] State Key Laboratory for Geo-mechanics and Deep Underground Engineering, School of Mechanics and Civil Engineering, China University of Mining and Technology, Xuzhou 221116, China
[b] Laboratory for Precision and Nano Processing Technologies, School of Mechanical and Manufacturing Engineering, The University of New South Wales, Sydney 2052, Australia
[c] Department of Safety Engineering, China Institute of Industrial Relations, Beijing 100048, China

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ABSTRACT

The nanosize grain growth characteristics of spherical single-crystal titanium oxide (TiO_2) during the rapid gaseous detonation reaction are discussed. Based on the experimental conditions and the Chapman–Jouguet theory, the Kruis model was introduced to simulate the growth characteristics of spherical TiO_2 nanoparticles obtained under high pressure, high temperature and by rapid reaction. The results show that the numerical analysis can satisfactorily predict the growth characteristics of spherical TiO_2 nanoparticles with diameters of 15–300 nm at different affecting factors, such as concentration of particles, reaction temperature and time, which are in agreement with the obtained experimental results. We found that the increase of the gas-phase reaction temperature, time, and particle concentration affects the growth tendency of spherical nanocrystal TiO_2, which provides effective theoretical support for the controllable synthesis of multi-scale nanoparticles.

Introduction

Because of its special properties, nanosize TiO_2 nanoparticles is widely used in industrial productions for many years. The characteristics of rapid, high temperature, and high pressure make gaseous detonation have become one way of preparing for nanomaterials, which has its special advantages, such as particles of high purity, good dispersion, small particle size, and weakly agglomeration. However, it is a lack of numerical simulation of nanosize grain growth via gaseous detonation. The speed of fuel mixture burning or detonation, supersonic velocity of the process, high temperature, and elevated pressure of the products have determined the engineering applications of the gaseous detonation reaction. The coupling between fluid dynamics and chemical energy release is the characteristic of detonation development (Liberman, 2008). Sustained by the elevated pressure and temperature owing to shock compression, chemical reactions continue and the detonation wave propagates. Detonation chemistry includes a strong impact, spontaneous heating, very fast chemical reaction rate and very short reaction time, and very narrow reaction zone. These characteristics quickly convert atom/molecule chemical energy into heat energy, while producing a strong shock wave, resulting in the reactants gasification, the formation of atom clusters or small mass species under the shock wave action. In the cooling process, the species or clusters reacting with each other can form nanoscale materials and new structures. This enables us to provide a novel, convenient, low operating cost, especially for carbon-based or nitrogen-based micro and nanomaterials synthesis pathway. Gaseous chemistry synthesis of nanomaterials (Kobata, Kusakabe, & Morooka, 1991; Li, Ouyang, Yan, Luo, & Mo, 2011; Ouyang, Li, Yan, Mo, & Zhao, 2008; Yan, Huang, & Xi, 2014) have made some progress, but in such extreme conditions, the growth characteristics of nanomaterials has been one of the problems that has troubled many researchers. The appropriate choice of particle growth model (Appel, Bockhorn, & Wulkow, 2001; Chen, Luo, Yan, & Liu, 2014; Kruis, Kusters, Pratsinis, & Scarlett, 1993; Kumar & Warnecke, 2010; Pourmehran, Rahimi-Gorji, Gorji-Bandpy, & Ganji, 2015; Wu, Nguyen, Flagan,

* Corresponding author at: State Key Laboratory for Geo-mechanics and DeepUnderground Engineering, School of Mechanics and Civil Engineering, China University of Mining and Technology, Xuzhou 221116, China. Tel.: +86 18305201191; fax: +86 051683590666.
E-mail addresses: nluo@cumt.edu.cn, ning.luo@unsw.edu.au (N. Luo).

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Nomenclature

a_0	monomer particle surface area ($m^{2)}$
a_p	aggregated surface area ($m^{2)}$
a_s	surface area of completely melt spherical particle ($m^{2)}$
C^0_{ni}	constant pressure heat capacity of the explosion reactant component i in the temperature T_0 (J/(mol K))
C^f_{ni}	constant pressure heat capacity of the explosion product component i in the temperature T_f (J/(mol K))
D_0	detonation velocity (km/s)
D_{CJ}	detonation velocity of CJ plane
D_d	particle diffusion factor
D_f	quality of the fractal coefficient
d_p	diameter of primary particle, m
e	specific internal energy of the reaction products (kJ)
e_0	specific internal energy of the solid explosive (kJ)
k_b	Boltzmann's constant (J/K)
N	number concentration of the particles (m^{-3})
n_i	amount of explosion product component (i)
n_p	primary particle number in an aggregated condition (m^{-3})
P_0	detonation pressure (Pa)
P_{CJ}	detonation pressure at the rear of the reaction zone (Pa)
Q	released specific heat from explosions (kJ/mol)
Q_p	heat of explosion at constant pressure (kJ/mol)
r_c	collision radius of the primary particle (m)
r_p	radius of the primary particle (m)
u_0	particle velocity (km/s)
u_{CJ}	particle velocity of CJ plane at the rear of the reaction zone (km/s)
υ	particle volume (m^3)
υ_0	monomer particle volume (m^3)
υ_p	aggregated particle volume (m^3)
ρ	density of gas-phase products (g/cm^3)
ρ_0	density of gas reactants (g/cm^3)
ρ_p	density of primary particle (g/cm^3)
γ	isentropic exponent
β	monodisperse collision frequency (cm^3/s)
τ	characteristic sintering time (s)
λ	mean free path of gas molecules

Okuyama, & Kousaka, 1988) to accurately predict the growth characteristics of the goal nanoparticles, which further reveals the growth mechanism of the goal nanoparticles under gaseous reaction, is still one of the problems in the research field. We attempt to use the classical Kruis model to predict the simulation of particle radius during the gaseous detonation process. Titanium dioxide is chosen to explore the feasibility of applying the model to detonation experiments. In this work, the Kruis model was introduced to simulate the growth characteristics of spherical TiO_2 nanoparticles based on the experimental conditions and the Chapman–Jouguet (CJ) theory. The numerical analysis results of sphere TiO_2 nanoparticles could show a satisfactory forecasting ability, which is different from the previous works. We preliminary report on the growth characteristics of spherical TiO_2 studied by numerical analysis based on the parameters of previous experimental conditions and results (Li et al., 2011; Luo, Chen, Liu, & Shen, 2013; Luo, Jing, Ma, & Yu, 2014), the rapid gaseous chemical reaction CJ theory and the Kruis model. The numerical analysis results of spherical TiO_2 nanoparticles show a satisfactory forecasting ability in comparison with the experimental results.

Theoretical study

CJ theory of the rapid gaseous chemical reaction

Detonations are rapid reactive wave phenomena whose propagation is controlled by shock waves. If the reaction rates are essentially infinite and chemical equilibrium is attained, a steady-state detonation is achieved whose propagation rate is governed solely by thermodynamics and hydrodynamics. In this paper, the steady-state detonation is discussed, which is distinctly different from flame combustion and other gaseous phase synthesized methods (Kho, Teoh, Mädler, & Amal, 2011; Zhou et al., 2013). Hence, the laws of conservation of mass, momentum, and energy applied across the shock front lead to the relations,

$$\rho_0 (D_0 - u_0) = \rho_{CJ} \left(D_{CJ} - u_{CJ}\right) \tag{1}$$

$$P_0 + \rho_0 (D_0 - u_0)^2 = P_{CJ} + \rho_{CJ} \left(D_{CJ} - u_{CJ}\right)^2, \tag{2}$$

$$e_0 + \frac{P_0}{\rho_0} + \frac{(D_0 - u_0)^2}{2} = e_{CJ} + \frac{P_{CJ}}{\rho_{CJ}} + \frac{\left(D_{CJ} - u_{CJ}\right)^2}{2} + Q, \tag{3}$$

$$\frac{P_{CJ} - P_0}{V_0 - V_{CJ}} = \gamma_{CJ} \frac{P_{CJ}}{V_{CJ}}. \tag{4}$$

In Eqs. (1)–(4), ρ is the gas density, D is the detonation velocity, u is the particle velocity, P is the detonation pressure, e is the specific internal energy, Q is the released specific heat from explosions, γ is the isentropic exponent, the subscripts 0 and CJ are respectively the physical quantities before and after rapid reaction. Internal energy e_i can be calculated from the following formula,

$$e_i = \frac{P_i V_i}{\gamma_i - 1}, \quad i = 0, \text{CJ} \tag{5}$$

Assuming that $\gamma_0 = \gamma_{CJ} = \gamma$, $P_0 \ll P_{CJ}$, so the result can be obtained,

$$D = \sqrt{2\left(\gamma^2 - 1\right) Q}, \tag{6}$$

$$P_{CJ} = \frac{\rho_0 D^2}{\gamma + 1}, \tag{7}$$

$$\rho_{CJ} = \frac{\gamma + 1}{\gamma} \rho_0, \tag{8}$$

$$u_{CJ} = \frac{D}{\gamma + 1}. \tag{9}$$

For the initial state under atmospheric pressure, the gas mixture can use the ideal gas equation of state, that is

$$T_{CJ} = \frac{P_{CJ} \rho_0}{P_0 \rho_{CJ}} T_0. \tag{10}$$

According to Hess's law, Q_p can be calculated from the following formula,

$$Q_p = \sum n_{\beta i} \Delta H^0_{f,\beta i} - \sum n_{mi} \Delta H^0_{f,mi}. \tag{11}$$

By the second law of thermodynamics,

$$Q_p = T_f \sum n_i C^f_{ni} - T_0 \sum n_i C^0_{ni}. \tag{12}$$

In Eqs. (11)–(12), Q_p is the heat of explosion at constant pressure, n_i is the amount of explosion product component i, C^f_{ni} is the constant pressure heat capacity of the explosion product component i in the temperature T_f, C^0_{ni} is the constant pressure heat capacity of the explosion reactant component i in the temperature T_0. So the