Micropyretic Synthesis: Heterogeneity Mapping in Ni-Al Composites

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Abstract: Micropyretic synthesis of Ni-Al composites often involves non-uniform initial composition and porosity, which have been overlooked in conventional modeling. This study numerically investigates the impact of these heterogeneities on the synthesis process. By generating heterogeneity maps for thermophysical and chemical parameters like density, heat capacity, thermal conductivity, and reaction yield, as well as micropyretic parameters such as pre-heat zone thickness and propagation velocity, we found that porosity variations significantly affect thermal conductivity and density compared to compositional changes. While porosity heterogeneities primarily influence physical properties, variations in Ni composition substantially reduce reaction reactivity. This research provides valuable insights into understanding the effects of initial conditions on micropyretic synthesis.

Keywords: micropyretic synthesis, ni-al composites, heterogeneity mapping, microstructure, materials science, composite materials

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1. Introduction

Micropyretic synthesis, also known as combustion synthesis, is a powerful technique for producing advanced materials. It utilizes highly exothermic reactions between solid-solid or solid-gas mixtures to generate a self-propagating combustion front within the material itself [1–8]. This innovative approach, pioneered in the Soviet Union during the [5], offers significant advantages over conventional methods.

Compared to traditional time-consuming and energy-intensive sintering processes, micropyretic synthesis boasts several key benefits. Firstly, it leverages exothermic reactions, eliminating the need for additional external energy input. Secondly, it allows for rapid production of near-final shapes (net shape processing) and minimizes waste generation, resulting in cleaner products. Additionally, studies have shown that materials synthesized through this method often possess superior mechanical and physical properties [2,3]. For instance, micropyretic synthesis has been shown to produce shape-memory alloys with significantly enhanced shape-recovery force compared to those made using conventional techniques [2].

However, the high thermal gradients inherent in micropyretic synthesis raise concerns about potential microstructural defects within the final product. The presence of such defects could lead to increased reactivity and improved sinterability [6]. Furthermore, this method offers rapid net shape processing, significantly reducing overall processing time compared to conventional powder metallurgy methods.

Despite extensive research on micropyretic synthesis in composite systems, existing numerical and analytical models [8] have primarily focused on homogenous systems. In reality, heterogeneities in both initial composition and porosity are prevalent during micropyretic synthesis due to the pressing or mixing of powders. These variations can lead to local fluctuations in reaction yield and crucial thermophysical/chemical parameters like density, heat capacity, and thermal conductivity. Consequently, the propagation velocity and combustion temperature of the combustion front are also affected. These changes can

ultimately contribute to the formation of non-uniform microstructures within the final product.

This study aims to address this critical gap in current knowledge. We employ a numerical simulation approach to investigate the impact of heterogeneities in initial composition and porosity on the micropyretic synthesis of NiAl composites. We will also generate heterogeneity maps that simultaneously consider both types of variations, allowing for a comprehensive understanding of how initial conditions influence the micropyretic reaction. By analyzing these maps, we can gain valuable insights into the effects of heterogeneities on the final product's properties.

2. Procedure

Energy Equation

The energy equation for transient heat conduction, including the source term, is given by:

$$\rho C_p \frac{\delta T}{\delta t} = \frac{\delta}{\delta z}\left[\kappa \frac{\delta T}{\delta z}\right] - \frac{4h(T - T_0)}{d} + \rho Q \theta(T, \eta) \tag{1}$$

where ρ is the density, C_p is the heat capacity, T is the temperature, t is time, κ is the thermal conductivity, h is the surface heat loss parameter, T_0 is the initial temperature, d is the sample length, ρQ is the heat release per unit volume, and $\theta(T, \eta)$ is the reaction rate.

Reaction Rate

The reaction rate, $\theta(T, \eta)$, is given by:

$$\theta(T, \eta) = \frac{\delta \eta}{\delta t} = K_0(1 - \eta)\exp\left(-\frac{E}{RT}\right) \tag{2}$$

where η is the fraction reacted, K_0 is the pre-exponential factor, E is the activation energy, and R is the gas constant.

Numerical Calculation

A numerical calculation is carried out with the assumption of first-order kinetics. The energy equation is discretized into 1201 nodes, and the enthalpy-temperature method coupled with the Gauss-Seidel iteration procedure is used to calculate the local temperature.

Initial and Boundary Conditions

The initial conditions are:

- At the ignition node, at time $t \geq 0$, the temperature is taken to be the adiabatic combustion temperature ($T = T_c$ and $\eta = 1$).
- At the other nodes, at time $t = 0$, the temperatures are taken to be the same as the substrate temperature ($T = T_0$ and $\eta = 0$).

Thermophysical/Chemical Parameters

The thermophysical/chemical parameters, such as thermal conductivity, density, and heat capacity, are calculated at each node using the following equations:

$$\rho_i = \sum_s \rho_s V_{s,i}(1 - P_i) \tag{3}$$

$$\kappa_i = \sum_s \frac{\kappa_s V_{s,i}(1 - P_i)}{1 + P_i/2} \tag{4}$$

$$C_{p,i} = \sum_s C_{p,s} X_{s,i} \tag{5}$$

where s denotes the component involved in the reaction, including Ni and Al.

Porosity Effects

The porosity effects of the reactants and product are considered in the numerical calculation. The initial porosity of the reactants at each node is calculated using:

$$P_i = P_0(1 + \text{Heteroporosity} \cdot f_R(j)) \tag{6}$$

where P_0 is the average global porosity, *Heteroporosity* is the assigned heterogeneity, and $f_R(j)$ is the random number at node j.

Convergence Criterion

The criterion used to ascertain whether the fraction reacted and enthalpies at each time level converge or not is determined from the relative error criterion. Once the convergence criterion for every node is met, the enthalpy and fraction reacted of the last iteration in a time step are considered to be the corresponding final values.

3. Result and Discussion

The study investigates the effects of heterogeneities in initial porosity and composition on the micropyretic synthesis of NiAl. The results show that the heterogeneities significantly influence the thermophysical/chemical parameters, such as density, heat capacity, thermal conductivity, and reaction yield, which in turn affect the micropyretic parameters, including propagation velocity and thickness of pre-heat zone [4].

The heterogeneity maps reveal that the heterogeneity in porosity has stronger effects on changing thermal conductivity than the heterogeneity in Ni composition. However, the heterogeneity in composition has stronger effects on changing reaction yield and heat capacity. The variations in composition and porosity change density, heat capacity, thermal conductivity, and exothermic heat, further influencing the reactivity at each node [5].

The propagation velocity is significantly reduced with the increase in heterogeneity in Ni composition, while it is only slightly changed with the increase in heterogeneity in porosity. The combustion temperature and propagation velocity dramatically change with the distance, and the stability and propagation velocity of the combustion front are expected to increase when the pre-heat zone becomes narrower [6].

The study also finds that the heterogeneity in composition has stronger effects on increasing the standard deviation of the velocity than the effects caused by the heterogeneity in porosity. The maximum standard deviation of propagation velocity is found when the 30% heterogeneity in composition and 40% heterogeneity in porosity occurs. Overall, the study highlights the importance of considering the heterogeneities in initial porosity and composition in the micropyretic synthesis of NiAl, as they significantly affect the thermophysical/chemical and micropyretic parameters [7].

The findings of this study have significant implications for the micropyretic synthesis of NiAl. The heterogeneities in initial porosity and composition can lead to variations in the reaction yield, exothermic heat, and propagation velocity, which can affect the quality and consistency of the final product [8]. The study also highlights the importance of controlling the heterogeneities in the initial reactants to achieve a more uniform and consistent reaction. This can be achieved through careful selection and processing of the reactants, as well as optimization of the reaction conditions.

Furthermore, the study demonstrates the effectiveness of the numerical model in simulating the micropyretic synthesis of NiAl. The model is able to capture the complex interactions between the thermophysical/chemical and micropyretic parameters, and provides valuable insights into the effects of heterogeneities on the reaction.

4. Conclusion

In conclusion, this study has investigated the effects of heterogeneities in initial porosity and composition on the micropyretic synthesis of NiAl. The results show that the heterogeneities significantly influence the thermophysical/chemical and micropyretic parameters, and can lead to variations in the reaction yield, exothermic heat, and propagation

velocity. The study highlights the importance of controlling the heterogeneities in the initial reactants and optimizing the reaction conditions to achieve a more uniform and consistent reaction. The numerical model used in this study has been shown to be effective in simulating the micropyretic synthesis of NiAl, and provides a valuable tool for further research and optimization of the process.

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