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Thermal Analysis of Preparation of Hydroxyapatite-$Ca(NO_3)_2$ and Na_3PO_4 Mixture Reaction Solution Based on Numerical Simulation

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A numerical model was presented to study the temperature distribution during the heterogeneous mixture reaction solution under microwave radiation. A case study of the preparation of hydroxyapatite, the electromagnetic field equations, fluid dynamics equations and heat transfer equations were solved by using finite-element method. The calculated results are in agreement with the experiments. The results show that the location of the hot spots is related to time and the hot spots often exist near the interfaces between the solution, solid and air.

Key Words: Thermal analysis, Hydroxyapatite, Numerical simulation.

INTRODUCTION

Most of the chemical reactions are sensitive to temperature; therefore using microwaves to heat reactants presents an impressive application prospect[1]. Unfortunately, some difficulties arose in the application of high-power microwaves in chemistry[2,3]. Furthermore, there are not any rigorous and effective methods to instruct the design of microwave chemistry reactor. Up to now, a number of efficient numerical approaches have been used to study the microwave heating. The coupled electromagnetic and thermal equations were used to study the microwave heating on water and food[4]. Huang method[5] based on experimental results was employed to study the microwave heating on homogeneous mixture reaction in a specially designed experimental system. However, many chemical reactions are heterogeneous. It was found that hot spots are often produced during the microwave heating on heterogeneous chemical reaction. A numerical model was presented to study the temperature distribution of heterogeneous mixture reaction solution under microwave radiation. A case study of the preparation of hydroxyapatite, the electromagnetic field equations, fluid dynamics equations and heat transfer equations were solved by using finite-element method. The calculated results were compared with the measured results. The agreement can be seen between the measured and calculated results. The results show that the location of the hot spots is related to time and the hot spots often exist near the interfaces between the solution, solid and air.

EXPERIMENTAL

Hydroxyapatite is a calcium phosphate compound $\{Ca_{10}(PO_4)_6(OH)_2\}$ that is frequently used as a bone graft material substitute due to its biocompatibility with bone[1] and its higher strength compared to other calcium phosphate compounds. Here, the reaction of preparation of hydroxyapatite using $Ca(NO_3)_2$ and Na_3PO_4 was considered.

In the above reaction, $Ca(NO_3)_2$ is 0.1 mol/L and Ca/P is 0.67. Modified Galanz700 microwave oven was used to heat on the reaction; frequency is 2450 MHz. Thermo view Ti30 was employed to measure the temperature. The construction experiment system is shown in Fig. 1.

RESULTS AND DISCUSSION

In the simulation of microwave heating on chemical reactions, we have to know the function of the effective permittivity with respect to temperature and reaction time. Generally, the effective permittivity of reactants changes with not only temperature but also reaction time. Here, the obvious bi-phases can be founded. The method can be employed to calculate the effective permittivity of the solution and deposition by means of genetic algorithms. By measurement, the effective permittivity

of solution and deposition both were hardly changed with time. So, the effective permittivities of solution and deposition were measured under the different temperatures and 2.45 GHz. For the solution and deposition, the measured effective permittivities at 2.45 GHz were shown in Fig. 2.

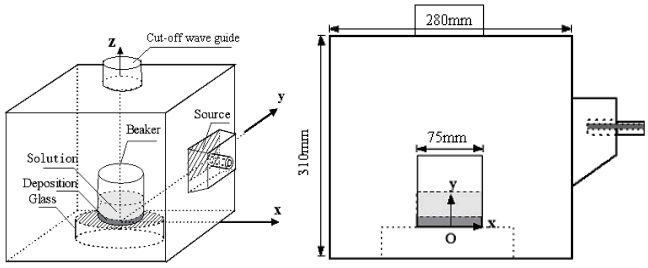


Fig. 1. Construction figure of experiment system

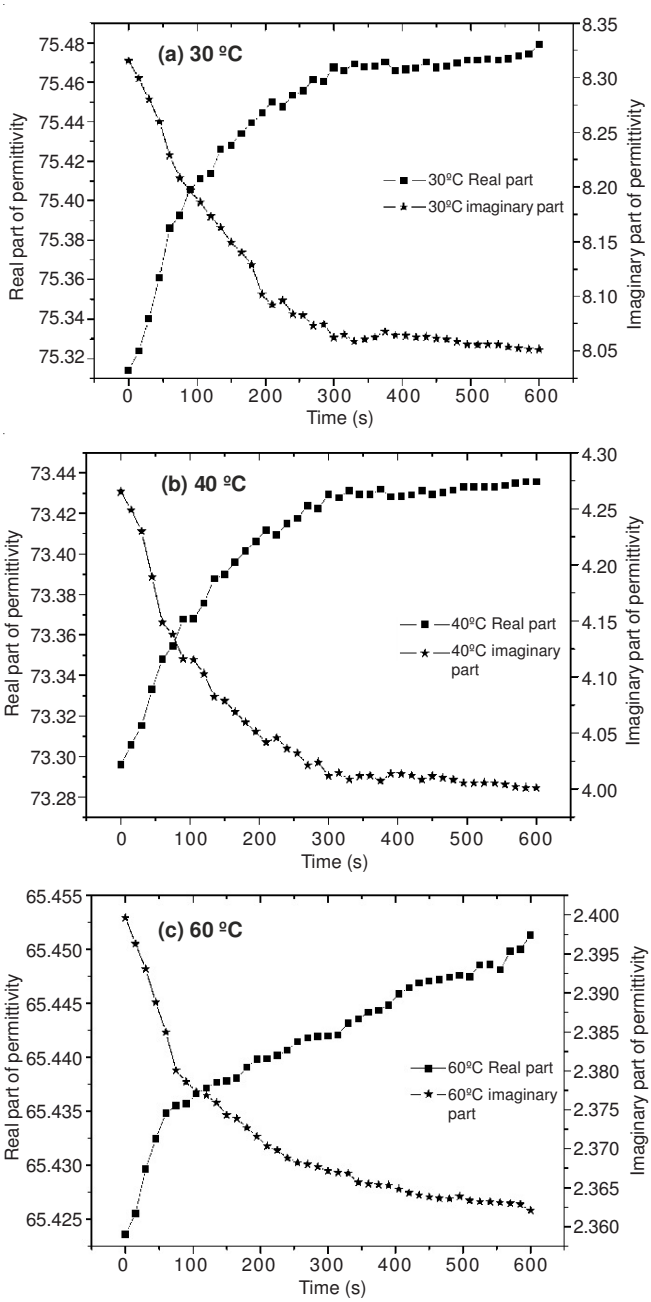


Fig. 2. Measured effective permittivities at 2.45 GHz

In order to analyze thermal properties during the preparation of nickel oxide reaction heated by microwave, the coupled Maxwell's equations, fluid field equations and heat transport equations were solved by using finite-element method. The flow chart of the numerical simulation of multiphysics is shown in Fig. 3.

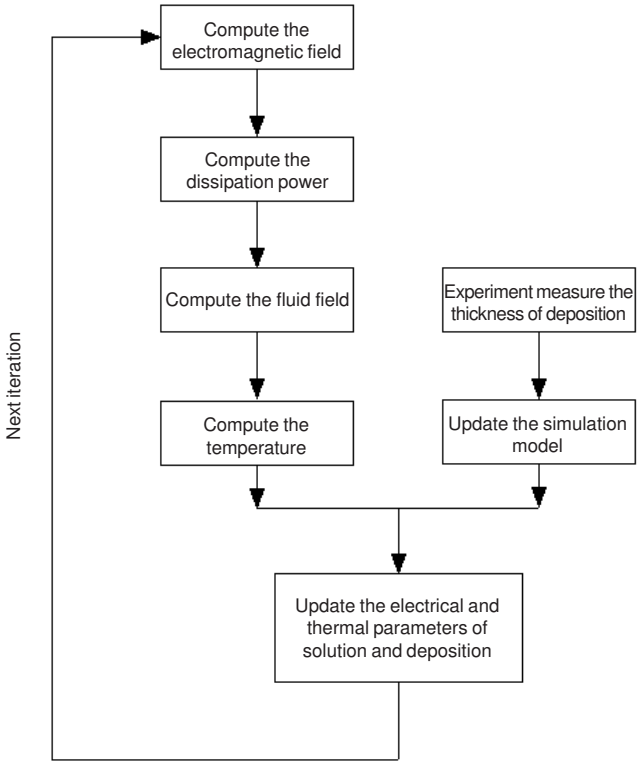
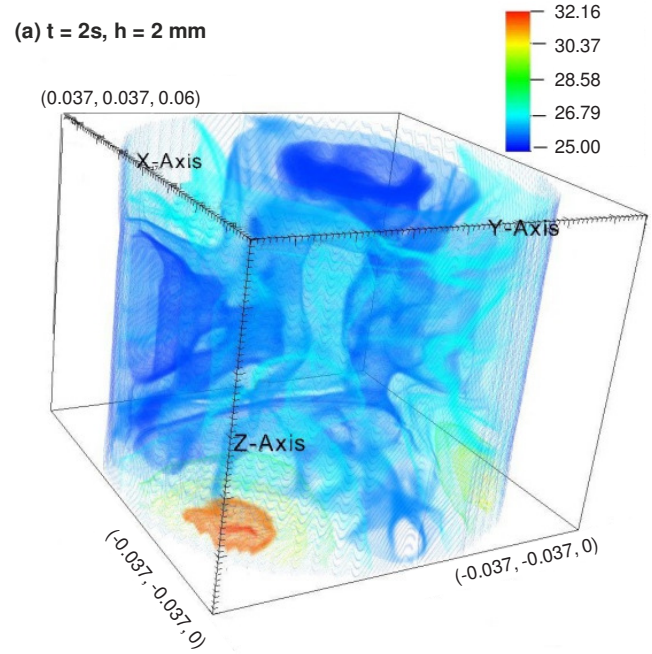


Fig. 3. Flow chart of the numerical simulation of multiphysics

By calculating, the resulted temperature distribution under the different time and thickness of deposition were shown in Fig. 4.



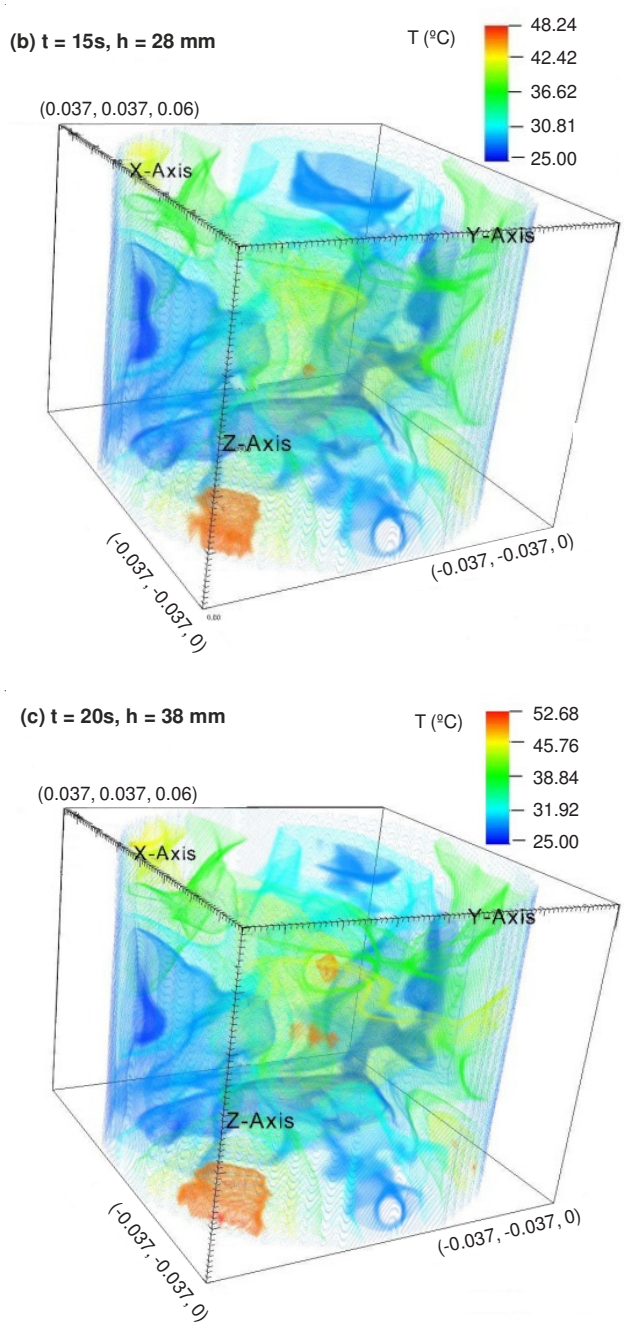
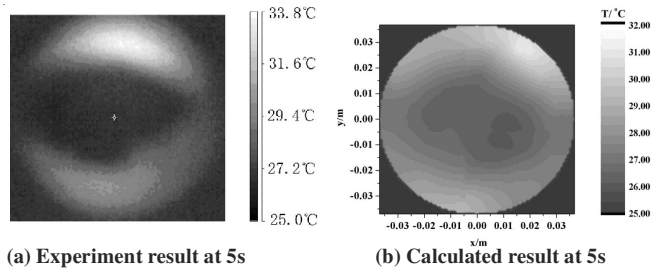


Fig. 4. Resulted temperature distribution under the different time and thickness of deposition

Additional, coordinate of the highest spots under the different heating time were shown in Table-1. To verity the calculated results, we repeat the above-mentioned experiment and use Thermo view Ti30 to obtain the distribution of temperature on the top interface of solution. The calculated and measured results are shown in Fig. 5.

TABLE-1

Heating time t (s)	Thickness l (mm)	Highness of the highest spots z = h (mm)
2	2.0	2.0
5	8.0	6.0
15	28.0	36.0
20	38.0	38.0



(a) Experiment result at 5s **(b) Calculated result at 5s**

Fig. 5.

Conclusion

The coupled electromagnetic field equations, reaction kinetics equations and heat transport equation solved to simulate the microwave heating on the hydroxyapatite. The measured temperature and calculated temperature are compared. Good agreement verifies the feasibility of the method. The results show that the location of the hot spots is related to time and the hot spots often exist near the interfaces between the solution, solid and air.

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REFERENCES

1. A. Loupy, Microwaves in Organic Synthesis, Wiley-VCH, Weinheim, 2002.
2. M. Chen, J.W. Hellgeth, E.J. Siochi, T.C. Ward and J.E. Mcgrath, *Polym. Engg. Sci.*, **33**, 1122 (1993).
3. J. Baker-Jarvis and R. Inguva, *J. Microwave Power Electromag. Energy*, **23**, 160 (1984).
4. H. Zhang and A.K. Datta, *J. Microwave Power Electromag. Energy*, **35**, 71 (2000).
5. S.G. Li, Y.Y. Koo, J.B. Wan, K.H. Young and V.V. Levdansky, *J. Chem. Eng. (Japan)*, **34**, 1567 (2001).