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FEM simulation and optimization on the elastic modulus and thermal expansion ratio of polymer-mineral composite

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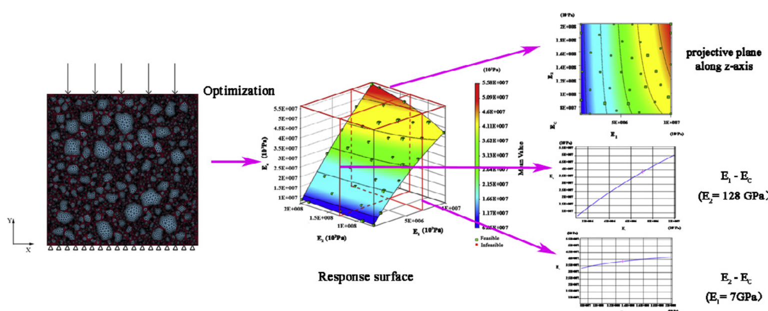
HIGHLIGHTS

- Finite element models of polymer-mineral composite are established.
- The composite's properties are optimized by Response Surface Methodology.
- Effects of components' properties on the composite's properties are investigated.

GRAPHICAL ABSTRACT



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ABSTRACT

In this research, the optimization on the overall properties of the polymer-mineral composite including the compressive elastic modulus and the thermal expansion ratio are investigated. The composite is simplified as a two-phase composite composed of coarse aggregates and matrix. 2D finite element model is built and verified by comparison with experimental results. The physical properties of the composite and components are set as responses and design variables respectively in the response surface methodology. Response surfaces reflecting how the components' physical properties influence the composite are obtained and analyzed, which is of significant importance in optimizing the composite's properties.

1. Introduction

Polymer-mineral composite material has been more and more widely used in the manufacture of machine tool beds for its superior workability, high strength-to-weight ratio, excellent damping characteristics, as well as low thermal conductivity and low thermal expansion coefficient [1,2]. However, its elastic modulus is lower than cast iron [3], so the machine structures made of polymer-mineral composite sometimes have insufficient stiffness to ensure the accuracy of precision machine tools. In addition, the meso-scale structure of polymer-mineral composite is heterogeneous [4], which may result in undesired nonuniform expansion and internal stress when ambient temperature changes, and finally have a negative impact on the precision level and machining speed of the end product. So it is of significant importance to investigate the effects of components on the composite's overall elastic modulus and thermal properties, and thus to optimize the design of the material structure and eventually to improve the material performance.

For simplicity, the polymer-mineral composite can be considered as a mixture of coarse aggregates and matrix that includes fine fillers and binder. Well-graded aggregates bonded together by matrix with excellent adhesion can improve the polymer-mineral

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composite's performance. Orak [5] carried out damping tests using polymer concrete and cast iron samples, and found out that polymer concrete was more appropriate than cast iron with respect to damping. Shokrieh [6] studied the effects of aggregate size, resin volume, as well as the percentage of chopped glass fiber on the mechanical properties, and an optimized polymer concrete with high strength was obtained. Martínez [7] discovered that the combination of medium and large particle sizes provides the highest elasticity modulus. But they did not consider the components' physical properties. Shigang [8] numerically simulated the effect of aggregates on the dynamic behavior of polyurethane concrete under tension by a finite element model, and the results showed that the aggregate shape had significant influences on the strength but no influence on the elastic modulus, while the thermal behavior of the material was not simulated. Lokuge [9] reported the effect of resin and fly ash contents on the strength of polymer mortar and polymer concrete. Yeon [10] performed laboratory testing and statistical analysis to identify the flexural fatigue performance of unsaturated polyester-methyl methacrylate concrete. Muthukumar [11] and Header [4] prepared specimens with different compositions of aggregates and resins, and investigated the mechanical properties under each mix proportion by experiments. However, the mixture-design based experiments just have very limited samples to test, and the individual or combined effects of each component's properties on the composites are very difficult to achieve.

In this paper, a 2D meso-scale numerical model for composites composed of aggregates and matrix is established. Numerical simulations are carried out by the finite element software LS-DYNA R7.0 [12], a widely used software in the modern industry applications for analyzing the large deformation static and dynamic response of structures. In the implicit solver, the equilibrium iterations can vary from problem to problem, so the cost per step is unknown since the speed depends mainly on the convergence behavior of the iterations. Non convergence is often resulted due to the inaccurate solution. Compared with the implicit solver, the explicit one has the better stability for the inexistence of equilibrium iteration and convergence problem. So explicit time integration, as the main solution method is employed in this research. What's more, specialization of the contact-impact algorithm can make the contact interfaces easily treated without the need of mesh transition regions, and varieties of element formulations are available for various element types.

There is seldom systemically optimization of the physical properties of polymer-mineral composite in the previous researches. In the conventional design approach, the best design is improved based on experience or intuition. It is basically choosing a better or best one from the predesigned and tested samples, but not a real parameter optimization. In this study, the optimization package LS-OPT 5.0, which is based on the Response Surface Methodology (RSM), is used to investigate the effects of aggregate and matrix's physical properties on the composite's overall properties including the compressive elastic modulus and thermal expansion ratio. Response surfaces reflecting how the components' properties influence the composite's behaviors are finally obtained in LS-OPT. The effects of both individual variables and their combination on the response are also discussed.

2. Construction of the 2D meso-scale finite element model

The method of building the numerical model has been introduced in our previous study [13]. The composite material is assumed to be a two-phase material composed of coarse aggregates and matrix. Inscribed polygons are firstly created based on the aggregate gradation, and randomly packed into a designated area. And then, convex or concave polygons which are similar to the real aggregate section shapes are generated by moving the polygon vertices inwards or outwards stochastically. Interference judgment among aggregate particles is applied to remove the overlapped polygons. Finally, the aggregates and matrix are meshed with triangles to generate the completed meso-structure. The meshing program, namely MESH2D, based on Delaunay triangulation, which best avoids triangulations with small angles among all possible triangulations of a set of points, is used in this paper. The node and edge information of aggregates and matrix are invoked to generate FE mesh. The obtained grid nodes and elements information are then exported to a K type of file for the sake of subsequent analysis.

The area distribution of the aggregate size is listed in Table 1. Considering the computation cost, the fine aggregates with dimension below 1.18 mm are neglected and regarded as the matrix combined with epoxy resin. A 2D meso-scale numerical model and a cross section image of real polymer-mineral composite material are shown in Fig. 1. The dimensions of the specimen are 100 mm × 100 mm. The aggregate, matrix and total element number of the numerical composite model are 62546, 67839, and 129385, respectively. And the generation time is 291.42 s.

3. Experimental procedures

The polymer-mineral composite used in this paper is assumed to be composed of coarse aggregates and matrix. The matrix is also a composite material including the epoxy resin, fillers and fine aggregates, whose physical properties should be obtained by series of experiments. The compressive elastic modulus of the polymer-mineral composite is also calculated by experimental procedures for the subsequent validity of the proposed numerical models. To reduce the experiment error, five groups of specimens are fabricated for each experiment to obtain the average value.

3.1. Determination of matrix mechanical properties

The matrix specimen is processed to dimensions (10 ± 0.2) mm × (10 ± 0.2) mm × (25 ± 0.5) mm by referring to GBT 2567-2008 to obtain its mechanical properties. Five matrix specimens used in the compression test are shown in Fig. 2.

The CMT4204 universal testing machine, which can computationally process and analysis the data, is employed in this study. The tested matrix specimen is positioned between the clamps, and loaded with a velocity 5 mm/min until failure occurs. The strain-stress curves of the five tested matrix specimens and a damaged matrix specimen are shown in Fig. 3.

The compressive elastic modulus E is calculated by:

$$E = \frac{L_0 \Delta P}{bh\Delta L} \quad (1)$$

where b and h are the specimen width and thickness respectively, L_0 is the initial height of specimen, ΔP is the load increment, and ΔL is the variation of specimen length corresponding to the increment of applied load.

The calculated compressive strength and elastic modulus of the five specimens as well as their average value μ and the Coefficient

Table 1
The aggregate size distribution of area.

Sieve size (mm)	Passing rate (%)
16.00	100.00
9.50	84.30
4.75	61.86
1.18	32.47