

Porous Cordierite Prepared by Emulsion Template Method Based on the First-Principles Calculation



Xuezhu Luan, Kaiyue Huang, Siyi Zhao and Jinhong Li

Abstract Porous cordierite ceramics (PCCs) were prepared by using emulsion template method using pure oxide as raw materials. The cell microstructures were constructed by the first-principle calculation. The thermal stability of cordierite was verified by the lattice vibration calculation at high temperature, band gap, and DOS. The microstructures and the effects of solid content on mechanical properties were investigated. PCCs with solid content of 40% had the uniform pore structure, which can be used in special industries.

Keywords Cordierite · First-principle calculation · Thermal stability · Porous structure · Solid content

Introduction

With the continuous improvement control of porous materials, the application fields and application scope of porous ceramics are also expanding [1, 2]. At present, its applications have spread to many scientific fields, such as environmental protection, energy saving, chemical industry, petroleum, smelting, food, pharmaceuticals, biomedicine, and so on [3–6]. The scientific fields of smelting, food, pharmaceuticals, and biomedicine have attracted the attention of global materials science [3–10]. Among them, porous cordierite ceramics (PCCs) can be used under relatively severe working conditions due to their extremely low thermal expansion coefficient and excellent thermal shock resistance, and become a common catalyst carrier material and high temperature and high pressure filter [11–16]. Currently, it is mainly made by artificial synthesis in industry. Compared with naturally occurring cordierite, synthetic cordierite has superior performance. With the

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continuous efforts of scientists for many years, porous cordierite ceramics have been developed to a great extent, and have achieved great economic and social benefits, but there are still several aspects to be further studied and improved [17–20]. Thermomechanical properties, the relationship between porosity and strength, precise control methods for pore size and shape distribution of materials, and reduction of production costs.

In this experiment, PCCs were prepared by using emulsion template method using pure oxide as raw materials. The microstructures and thermal stability were determined by first-principles calculation. The effects of solid content on mechanical properties were investigated.

Experiments

Commercially available materials, magnesia (AR, Sinopharm Chemical Reagent Co., Ltd. Shanghai, China), alumina (AR (analytical reagent), Xuancheng Jingrui New Material Co., Ltd. Anhui Province, China), and silica (AR, Shenzhen Crystal Materials Chemical Co., Ltd. Guangdong Province, China), were blended together to obtain ceramic suspensions and were ball milled for 12 h with ZrO₂ balls (10 mm), 2.0 wt% ammonium polyacrylate salt (Adamas Reagent Co., Ltd.), 0.5 wt% PVA (AR, Adamas Reagent Co., Ltd.) and different addition of mullite fibers (Beijing Chemical Works). Afterward, 2.0 wt% propyl gallate (C₁₀H₁₂O₅) (AR, Adamas Reagent Co., Ltd.) was dissolved in ethanol (AR, Beijing Chemical Works) and added to suspended particles, until arriving an in situ modified state [21]. Then, octane (200 vol%, AR, Beijing Chemical Works) was added to the suspension, followed by the emulsification process under continuous stirring by an electric mixer (HR1613, Philips) at full speed for 5 min. Finally, all the emulsions were transferred to culture vessels (2 cm in height and 9 cm in diameter) and dried at room temperature. After oil and water evaporate, the dried samples were shaped. Finally, the samples were sintered at different temperatures for 2 h. The morphology was observed by scanning electron microscopy (SEM, S4800, Hitachi, Japan). The pore size distribution of the samples was evaluated by mercury intrusion porosimeter (PoreMasterGT60, Quantachrome).

Results and Discussion

The energy band theory is a major theoretical basis for studying microscopic motion. It is based on the viewpoint of quantum mechanics, so that individual electrons in a solid are no longer bound to individual atoms, but move throughout the whole solid. Although the single electron theory is an approximation theory, its actual development proves that it has become the basis for accurately summarizing the laws of electron motion in some important fields. The band theory divides

crystals into metals, semiconductors, and insulators according to electrical properties. It not only explains the conductive properties of the crystal but also explains the optical, magnetic, and thermal properties of the crystal. The energy band structure calculated by the first principle can explain the difference between metal, semiconductor, and insulator. When the band gap is 0 eV or very small, the solid is a metal material, and electrons can easily obtain energy at room temperature and transition to rewinding to conduct electricity. When the band gap is greater than 9 eV, it is an insulating material, and it is difficult for electrons to transition to the conduction band, and thus it is impossible to conduct electricity. The semiconductor material has a band gap of 1–3 eV between the conductor and the insulator. As shown in Fig. 1, the cordierite microstructure was closely combined by SiO_2 , Al_2O_3 tetrahedron and MgO octahedron, and the gap of the band gap was 4.6875 eV. The band length was a transition, so cordierite had a stable structure. As shown in Fig. 2, it can be seen from the state density analysis that the DOS state had the X-axis symmetry characteristic and belong to the semiconductor or insulator, which further verified the thermal stability of cordierite. It can be seen from Fig. 3 that the microstructure of cordierite was calculated at high temperature, and its microstructure did not change at room temperature and high temperature of 1300 °C, so cordierite had excellent high-temperature resistance.

The effect of different solid contents on the morphology of PCCs is shown in Fig. 4. When the solid content was 20%, the particles and particles cannot be bridged together because of fewer solid particles. When the oil phase was removed, the spherical structure collapsed to form an irregular macroporous structure. With the increase of solid content, the pore structure tended to be uniform. When the solid content was 40%, the porous structure with uniform pore size distribution was formed, and PCCs were formed by high temperature sintering. As shown in Fig. 5, the pore wall became thinner after high temperature sintering. Cordierite, as rod-like particles, was arranged on the pore wall after high temperature sintering to

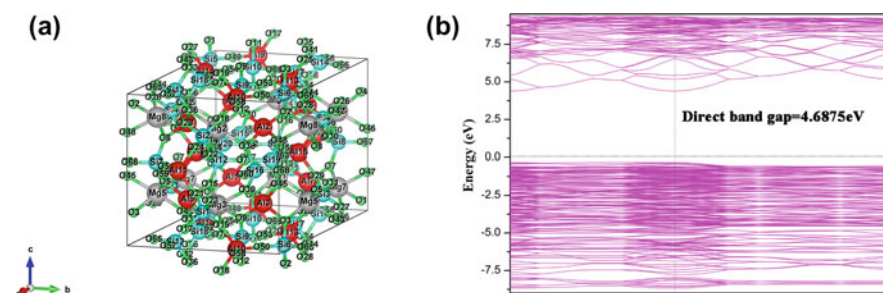


Fig. 1 a Cellular structure b Band gap of cordierite based on first-principles calculation

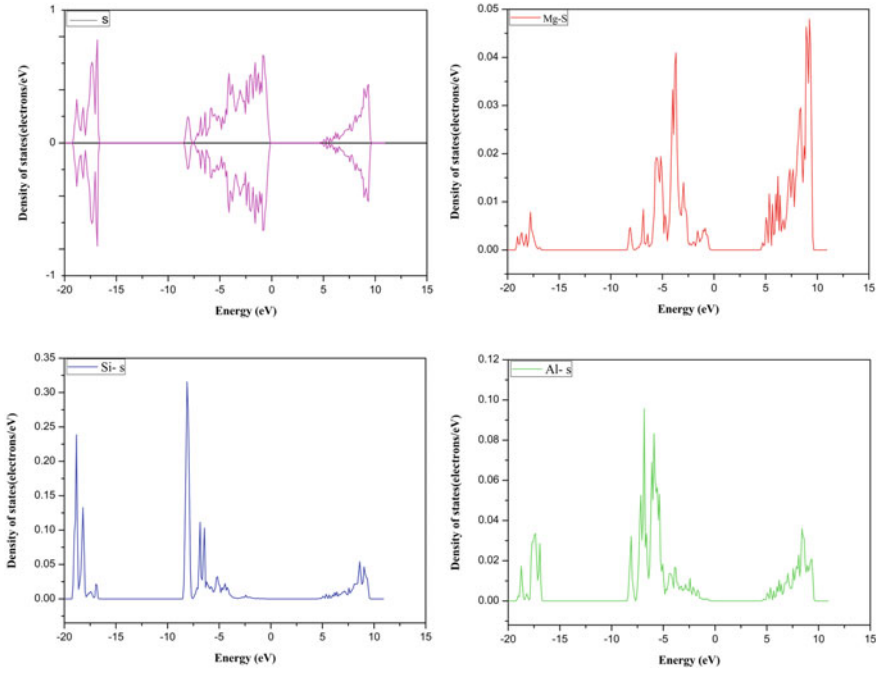


Fig. 2 DOS of cordierite

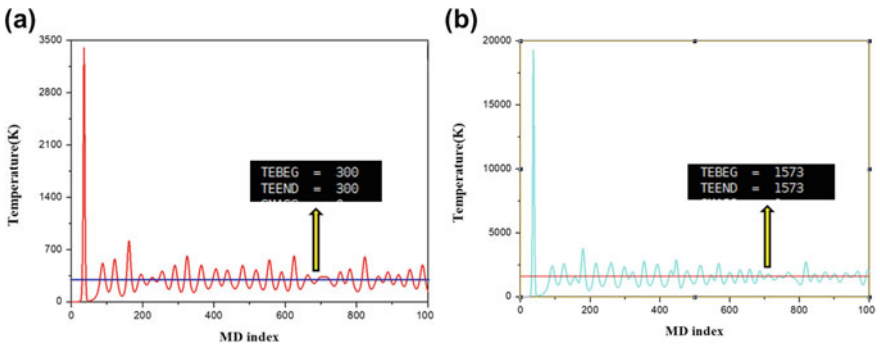


Fig. 3 First-principles calculation of cordierite at high temperature

form porous structure. The strength of PCCs is mainly determined by the properties of the products. The second impurity phase will not appear by pure oxide as raw materials. Cordierite as the main crystal phase can improve its thermal stability and the mechanical strength.

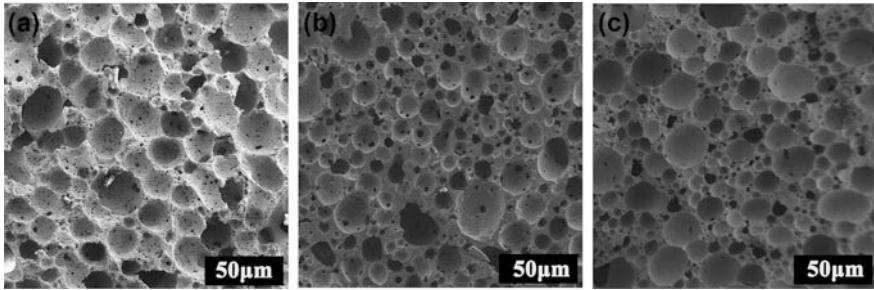


Fig. 4 The effect of different solid contents on the morphology of PCCs **a** 20%, **b** 30%, **c** 40%

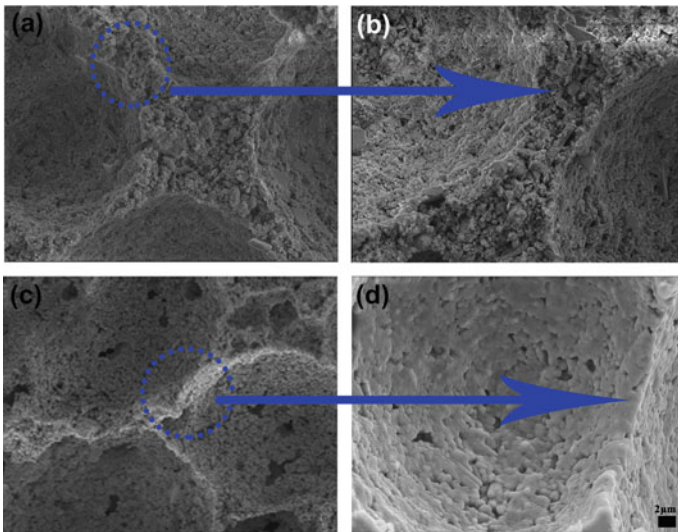


Fig. 5 SEM images of PCCs at different temperatures **a** 0 °C, **b** pore wall at 0 °C, **c** 1300 °C, **d** pore wall at 1300 °C

Conclusions

In this experiment, PCCs were prepared by using an emulsion template method using pure oxide as raw materials. The first-principle calculation was used to construct the cell microstructures to verify its excellent properties. Its stability was verified by band gap. DOS verified its non-conductivity. The thermal stability was verified by the lattice vibration calculation at high temperature. The microstructures and the effects of solid content on mechanical properties were investigated. PCCs with solid content of 40% had the uniform pore structure, which can be used in special industries.

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