The Solid-Phase Method Synthetics and Study the Thermoelectric Properties Analyze of $Ca_3Co_2O_6$

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***Abstract*—Used $CaCO_3$ and Co_2O_3 as raw materials of the Experiment, which successfully synthesized $Ca_3Co_2O_6$ *thermoelectric* material by solid-phase method. Study the morphology and microstructure by X-ray diffraction pattern (XRD) and scanning electron microscopy (SEM), the results show that the forming temperature of $Ca_3Co_2O_6$ is 900℃, and not form other impurities at 900℃, when the temperature rise to 1000℃, the $Ca_3Co_2O_6$ decomposed into CaO. The SEM analysis results shows that the morphology of $Ca_3Co_2O_6$ is a worm-like curled up, formed at 900℃.**

***Index Terms*—$Ca_3Co_2O_6$, Solid-phase method, thermoelectric material, forming temperature**

I. Introduction

Recently, with the development of the society the environment is destruction, the energy is shortage, and the people is face with the severe environment problem and energy crisis. So looking for thermoelectric material is becomes the study focus [1]-[3]. The thermoelectric material $Ca_3Co_2O_6$ has good thermal chemical properties and chemical stability [4]-[6], can applicable to work under the extreme environment and has great application potential at the high thermoelectric field [7]-[8]. It makes up the defects of the metal compounds thermoelectric material that was oxidized and corroded at high temperature environment. The $Ca_3Co_2O_6$ material was formed by Helmer and Fjellvag and was studied as thermoelectric material in 1995 [9]. The single-crystalline and polycrystalline of $Ca_3Co_2O_6$ have been formed using molten salt method and solid phase method by M. Mikmai [10]. The results of conduction properties show that the grain boundary resistance and anisotropic leads to resistivity of polycrystalline is the 10-100 times than single crystal [11]. The ZT of $Ca_3Co_2O_6$ is 0.15 at 800℃ this is beneficial to improve the thermoelectric properties. The band energy structure and thermoelectric of $Ca_3Co_2O_6$ have studied by Nan Wence, the results show that the disintegrate temperature is 1026 ℃, and $Ca_3Co_2O_6$ was decomposed completely at 1050℃, the decomposed product were Co_3O_4 and CaO. In this paper, the $Ca_3Co_2O_6$ thermoelectric materials was synthesized by solid phase method, the main raw materials are $CaCO_3$ and Co_2O_3.

II. Experiment

(1)Take $CaCO_3$ and Co_2O_3 according to the stoichiometry of $Ca_3Co_2O_6$.

(2) Fully grinding the power of $CaCO_3$ and Co_2O_3 in the mortar, the grind time is 1h.

(3) The power which is fully grinding put in the four crucibles, and the sintering temperature of four crucibles are 700℃, 800℃, 900℃ and 1000℃ respectively.

(4) The flow diagram of muffle furnace temperature was shown in Fig. 1.

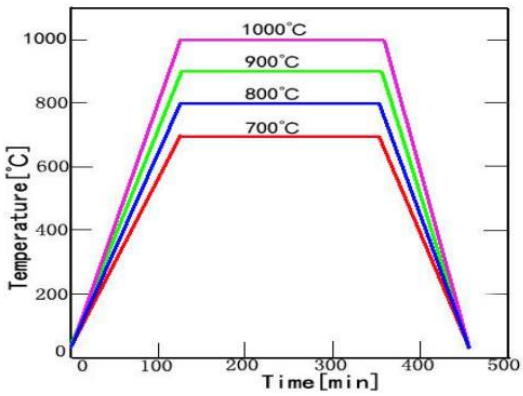

Figure 1. The flow diagram of muffle furnace temperature

III. The Experimental Results and Discussion

A. The XRD Analysis Results of the Sample $Ca_3Co_2O_6$

The X-ray diffraction (XRD) is applied to analyze the lattice parameter and phase structures. The Fig. 2 is the XRD of the sample $Ca_3Co_2O_6$, the work voltage is 45KV, the work current is 30mA.In this figure the curve are show the peak value of the sample composition, the calcinations temperature is 900℃ and 1000℃, respectively. The analysis results show that the pure $Ca_3Co_2O_6$ was formed at 900℃, the position of the sample composition peak and the $Ca_3Co_2O_6$ XRD curve

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of JCPDS (00-051-0311) standard calorie are consistent. When the sintering temperature rise to 1000℃, $Ca_3Co_2O_6$ is decomposed into CaO.

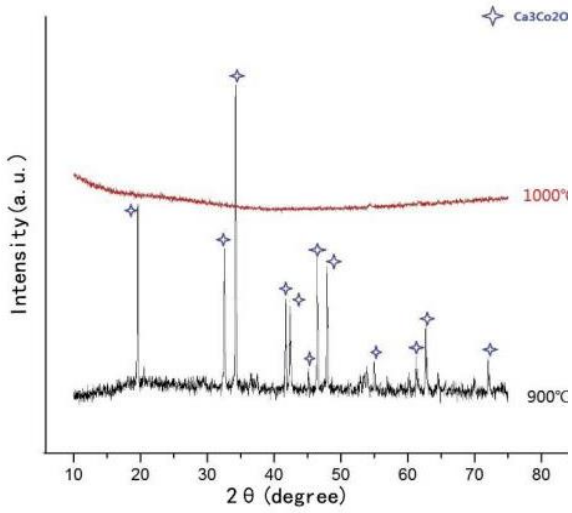
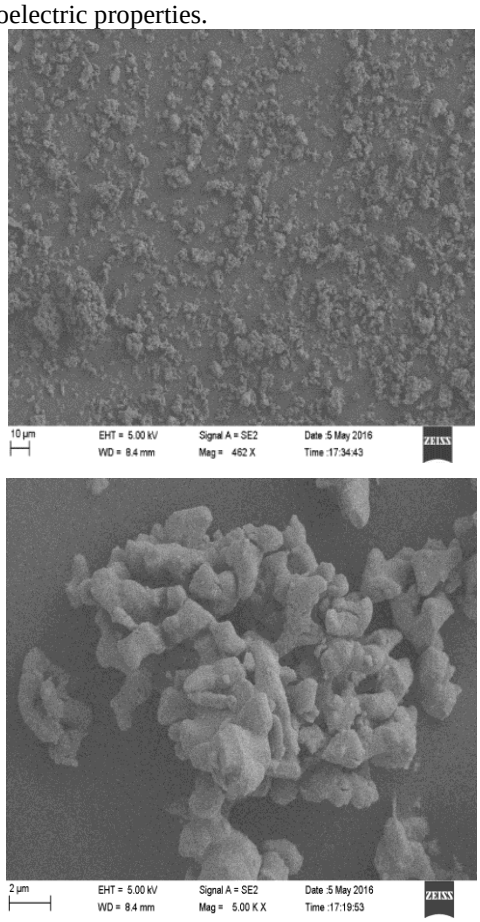


Figure 2. The XRD analysis results of the sample $Ca_3Co_2O_6$

B. The SEM Analysis Results of the Sample $Ca_3Co_2O_6$

The Scanning Electron Microscopy, (SEM) is applied to analyze the material morphology and microstructure. The Fig. 3 is the SEM of the sample $Ca_3Co_2O_6$ (the calcinations temperature was 900℃). The result shows that the grain of crystal morphology distribution is uniform, and the morphology of $Ca_3Co_2O_6$ is a worm-like curled up, it conduce to improve the thermoelectric properties.



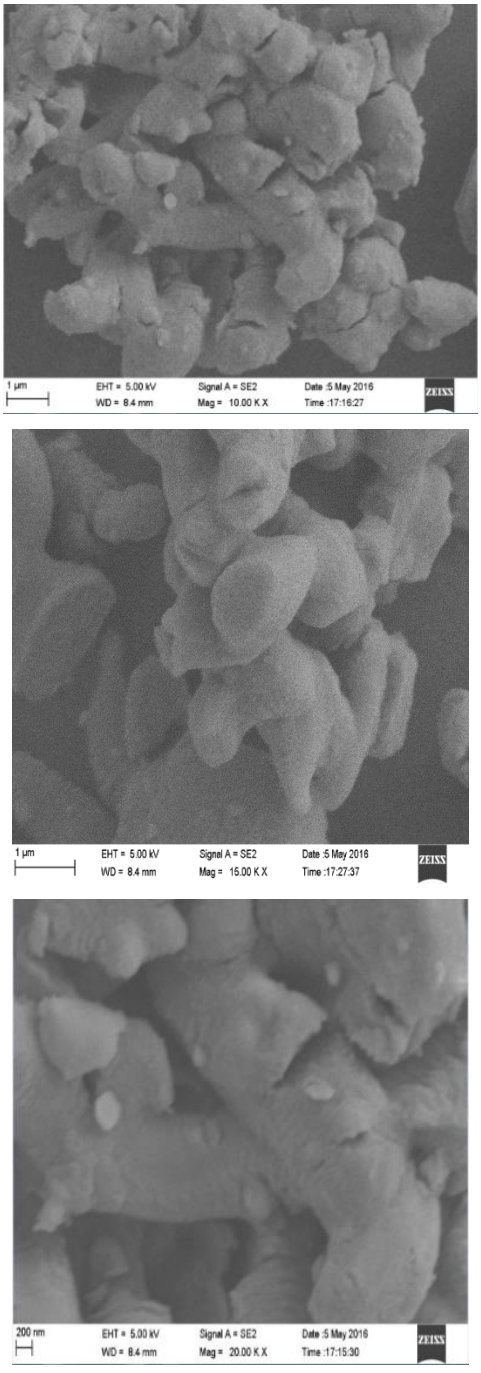


Figure 3. The SEM analysis results of the sample $Ca_3Co_2O_6$

IV. Theoretical Calculation

The Fig. 4 is the theoretical model of $Ca_3Co_2O_6$, the result show that $Ca_3Co_2O_6$ along to trigonal crystal, each cell has 12 atoms of which 6 Ca atoms, 4 Co atoms and 12 O atoms. The lattice constant of a, b and c are 9.061, 9.061 and 10.367, respectively. The result is match well with the literature [12].

The Fig. 5 is the crystal morphology of $Ca_3Co_2O_6$, the calculation results shows that the crystal morphology of $Ca_3Co_2O_6$ is trigonal dodecahedron crystal, the results is match well with the SEM.

The Fig. 6 is the density of states of $Ca_3Co_2O_6$, the result shows that the density states of $Ca_3Co_2O_6$ is

contributed from the Ca 3p 3d, Co 3d and O 2p near the Fermi surface, and in the valence band the density states are from the Ca 3p 3d and Co 3d, in the conduction band the density states is from O 2p. When the electric energy far away the Fermi surface, the density states is become little, the result provide the theoretical support for the emitting mechanism analysis.

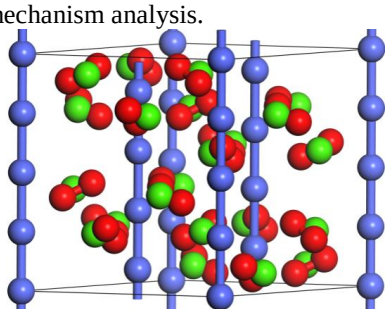


Figure 4. The theoretical model of $Ca_3Co_2O_6$

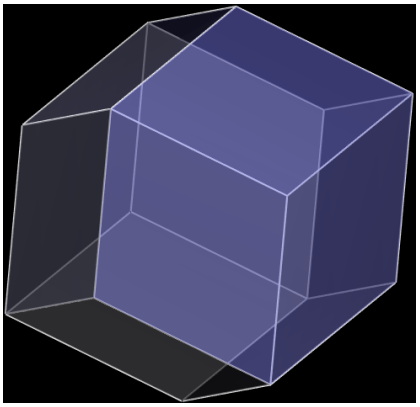
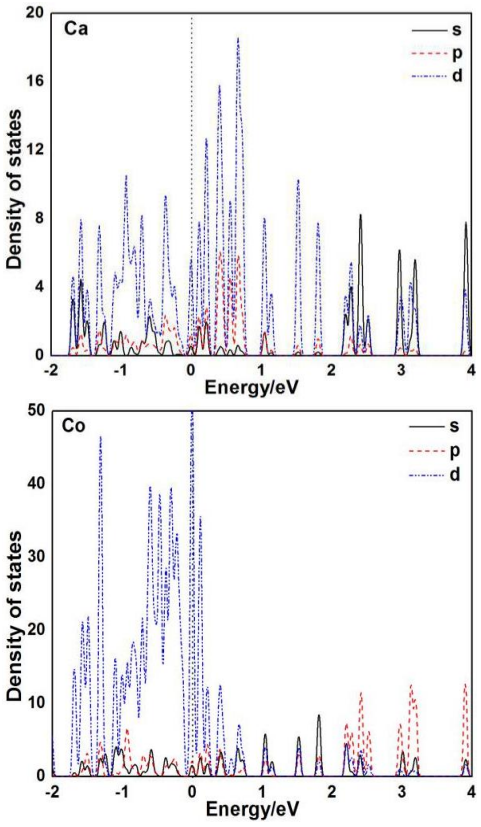


Figure 5. The crystal morphology of $Ca_3Co_2O_6$



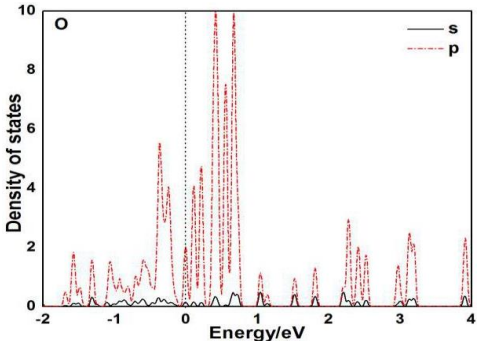


Figure 6. The density of states of Ca_3Co_2O

V. CONCLUSIONS

Based on $CaCO_3$ and Co_2O_3 as raw materials forming the $Ca_3Co_2O_6$ material compound using solid-phase method, and analyze the crystal structure. The results show that that the forming temperature of $Ca_3Co_2O_6$ is 900℃, and not form other impurities at 900℃, when the temperature rise to 1000℃, the $Ca_3Co_2O_6$ decomposed into CaO. The SEM analysis results shows that the morphology of $Ca_3Co_2O_6$ is a worm-like curled up, formed at 900℃.

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