Structures and Photoelectric Properties of Ce and Co Doped CuInTe₂ Semiconductor

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Keyword: CuIn₁₋ₓ₋ₐₓ₋ₜₓ₋ₕₓ₋ₜₓ₋ₙₓ₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋₅0.1, y=0, 0.1, 0.2 and 0.3), which the raw materials (Cu, In, Ce, Co, Te ) purity were higher than 99.99%, were synthesized by vacuum arc-melting method. Considering the volatility of tellurium, an extra 10% of Te was added for compensating the weight losses during the melting. To ensure the homogeneity, each sample was turned upside and down for 3 times. The phase structure were checked using an X-ray diffractometer (Rigaku G/max 2500, using CuKa1 radiation with λ=1.54056Å; 40m A, 200Kv). The field emission scanning electron microscopy (FE-SEM JSM-7001F) equipped were used to investigate the surface morphologies. The absorption rate dependence of wavelength for CuIn₁₋ₓ₋ₐₓ₋ₜₓ₋ₙₓ₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋ₜ_x₋₅0.1, y=0, 0.1 and 0.3) was obtained on a Shimadzu 2450UV-Vis spectrophotometer.

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Results

XRD Analysis

The X-ray Diffraction (XRD) of CuIn$_{1-x-y}$Ce$_x$Co$_y$Te$_2$ (x=0.1, y=0, 0.1, 0.2 and 0.3) are shown in Fig.1. The diffraction peaks could be indexed as a tetragonal structure according to the result of TREOR program. The planar indices follow the extinction laws of the chalcopyrite CuInTe$_2$ with a space group of I-42d. The diffraction characteristic peaks of (112), (220), (312), (316) and (424) planes in the chalcopyrite structure are observed for CuIn$_{1-x-y}$Ce$_x$Co$_y$Te$_2$ samples. The lattice parameter of the samples also be calculated and the results are revealed in Fig.2 (a)-(b). The lattice parameters and volumes are corresponding to a= 6.1901Å-6.1951Å, c=12.3217Å-12.4293Å. We can see that lattice show fluctuation phenomenon which may be the influence of the impure phase CoTe$_2$ and CeO$_2$.

![Fig.1 XRD Patterns of CuIn$_{1-x-y}$Ce$_x$Co$_y$Te$_2$ Samples](image)

![Fig.2 Latter Parameters a (a) and c (b) Dependence of Co Contents](image)

SEM Analysis

The Cerium and Cobalt content dependences of SEM morphologies for CuIn$_{1-x-y}$Ce$_x$Co$_y$Te$_2$ (x=0.1 and y=0, 0.1, 0.3) are shown in Fig.4 (a)-(c), respectively. It can be seen in the three follow picture that the growths of the grain is inhomogeneous with the distribution of both lager bulks and small pieces. The grain sizes tend to decrease with the increase of Co content in CuIn$_{1-x-y}$Ce$_x$Co$_y$Te$_2$ semiconductor. The morphologies on the grain surfaces show that the evolutions of the grains from initial columnar crystal to larger granularity with cuspidal particals and the finally layer structures.
Fig. 3 SEM Images of CuIn_{0.9-y}Ce_{0.1}Co_{y}Te_2 (y=0-0.3) Powders

Absorption Performance

Fig. 4 UV-Vis Spectra of CuIn_{0.9}Ce_{0.1}Te_2, CuIn_{0.8}Ce_{0.1}Co_{0.1}Te_2 and CuIn_{0.6}Ce_{0.1}Co_{0.3}Te_2 Powders
The absorption spectra of CuIn$_{0.9-y}$Ce$_{0.1}$Co$_y$Te$_2$ recorded by UV-vis spectrophotometer at room temperature with the wavelength between 400nm-800nm. And the curve is shown in Fig.4.

The direct band gap ($E_g$) can be calculated by the equation (1)$^{[8]}$:

$$\alpha(h\nu) = A/h\nu (h\nu - E_g)^p$$

where $\alpha$ is the absorption coefficient, $A$ is a constant and $p$ depends on the nature of transitions, $p=1/2$ for direct transitions and $p=2$ for indirect transitions. The picture of $(\alpha h\nu)^2$ versus $h\nu$ is shown in Fig.4. From the extrapolation of the curve to $(\alpha h\nu)^2=0$, the energy gap of the CuIn$_{0.9}$Ce$_{0.1}$Co$_y$Te$_2$ ($x=0.1$ and $y=0,0.1,0.3$) is calculated to be 1.17eV for CuIn$_{0.9}$Ce$_{0.1}$Te$_2$, 1.20eV for CuIn$_{0.8}$Ce$_{0.1}$Co$_{0.1}$Te$_2$ and 1.27eV for CuIn$_{0.6}$Ce$_{0.1}$Co$_{0.3}$Te$_2$, respectively. It can be seen that the energy band gap increases due to the increase of Co content.

Conclusions

Cerium and Cobalt doped CuInTe$_2$ powders were successfully synthesized by vacuum arc-melting. XRD shows that CuIn$_{1-x-y}$Ce$_x$Co$_y$Te$_2$ ($x=0.1$, $y=0,0.1,0.2$ and $0.3$) have a tetragonal chalcopyrite structure and the space group is I-42d. The lattice parameter shows fluctuation phenomenon because of the influence of the impure phase. SEM morphologies of the samples indicate that the grain sizes tend to decrease with the increase of Co content. UV-Vis measurements demonstrate that increase of Cobalt content can raise the energy band gap of the samples. It is more suitable for the absorbed layer material solar spectra than CuInTe$_2$.

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References

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