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## **Studies on CrSi<sub>2</sub> Nanocrystal Encapsulated with Styrene / Acrylonitrile Copolymer**

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CrSi<sub>2</sub> nanocrystals, prepared by the method of direct arc plasma, were encapsulated with the styrene/acrylonitrile copolymer. X-ray powder diffraction (XRD) pattern and Raman spectra of the composite proved the successful encapsulation. Transmission electron microscopy (TEM) image showed that the CrSi<sub>2</sub> nanocrystals were dispersed in copolymer matrix homogeneously.

**Keywords:** CrSi<sub>2</sub> Nanocrystal; Copolymer; Encapsulation

### **INTRODUCTION**

Semiconductor nanocrystals have given rise to extensive attention due to their excellent optical, electrical and chemical properties.<sup>1</sup> In order to put them into practical application, one promising way is to encapsulate them with copolymer, which will improve their assembled and manipulated capability greatly.<sup>2</sup> CrSi<sub>2</sub> is an excellent p-type semiconductor with a direct band gap of 0.34 eV.<sup>3,4</sup> However, CrSi<sub>2</sub> nanocrystal prepared by the direct arc plasma method is generally in aggregating state and also difficult to be assembled further. In order to overcome this problem, we attempt to encapsulate CrSi<sub>2</sub> nanocrystal with styrene/acrylonitrile copolymer. The

characterization on the composite with TEM, XRD and Raman spectra proved the successful encapsulation.

## EXPERIMENTAL SECTION

### The Preparation of CrSi<sub>2</sub> Nanocrystal

CrSi<sub>2</sub> can be prepared by reacting silicane with the vapor of Chromium. In our experiment, metal Chromium was evaporated into the silicane atmosphere by the direct arc plasma discharge, the subsequent reaction led to the formation of CrSi<sub>2</sub> nanocrystal.

### The Preparation of Copolymer

The styrene/acrylonitrile random copolymer was prepared by radical polymerization using azobisisobutyronitrile as an initiator. Its molecular weight was about 12,000, and the content of nitrile group was about 9%.

### CrSi<sub>2</sub> Encapsulated with Copolymer

The styrene/acrylonitrile random copolymer was dissolved in tetrahydrofuran with a trace of CCl<sub>4</sub>, followed by the addition of CrSi<sub>2</sub> powder. The reaction was facilitated by ultrasonic agitation. After removal of the suspended CrSi<sub>2</sub>, a yellow solution containing CrSi<sub>2</sub>/polymer composite was obtained.

## RESULTS AND DISCUSSION

Fig. 1 shows the XRD pattern of CrSi<sub>2</sub> nanocrystal. Two strong diffraction peaks appear at 43.0° and 49.7°, respectively, which correspond to the (111) and (112) characteristic diffraction of CrSi<sub>2</sub>. And a shoulder peak at 42.4° can be assigned to its (003) characteristic diffraction. From these peaks, we

could determine the average size of  $\text{CrSi}_2$  nanocrystal to be 20 nm by the Scherer's formula:  $D = k \lambda / \beta \cos \theta$  ( $D$  is the size of nanocrystals,  $\lambda$  is the wavelength of X-ray, and  $\beta$  is the half width of the peak). However, from the TEM image we couldn't determine the size of  $\text{CrSi}_2$  particles, since they are aggregated seriously.

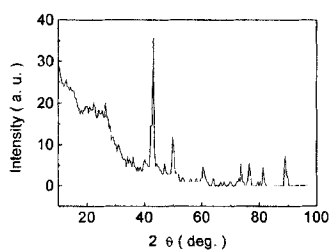


FIGURE 1 XRD pattern of  $\text{CrSi}_2$  nanocrystal.

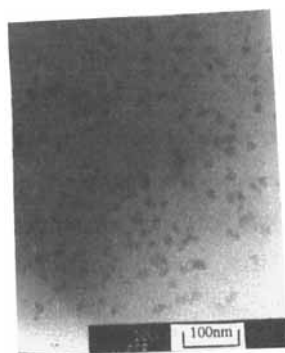


FIGURE 2 TEM image of  $\text{CrSi}_2$  capped with copolymers.

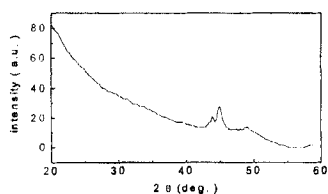


FIGURE 3 XRD pattern of  $\text{CrSi}_2$  nanocrystal capped with copolymers.

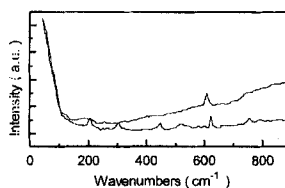


FIGURE 4 a: Raman spectrum of nanocrystal capped with copolymers. b: pure copolymers.

After encapsulated with styrene/acrylonitrile random copolymer,  $\text{CrSi}_2$  nanocrystal was dispersed into copolymer homogeneously and didn't form the aggregation, as shown in Fig. 2. The average size of the particles can be determined to be 25 nm from it, which is consistent with the XRD result shown above. Fig. 3 shows the XRD pattern of  $\text{CrSi}_2$ /copolymer composite,

the characteristic peak of  $\text{CrSi}_2$  nanocrystal at  $42.4^\circ$  and  $43.0^\circ$  can still be observed, which also prove the successful encapsulation. But, other characteristic diffraction of  $\text{CrSi}_2$  were indistinguishable due to the strong scattering of polymer.

Fig. 4 depicted the Raman spectrum of  $\text{CrSi}_2$ /copolymer composite (curve a) and pure copolymer (curve b). Compared with the two curves, we can find that some new peaks appear in the composite. The band located at  $307.17\text{cm}^{-1}$  is the characteristic vibration of Cr-Si bond, which is red-shifted  $3\text{ cm}^{-1}$  compared to the bulk  $\text{CrSi}_2$  due to the surface encapsulation. The band at  $446.7\text{cm}^{-1}$  can be attributed to the new surface phonon vibration mode of  $\text{CrSi}_2$  nanocrystal caused by the surface passivation of polymer. While the bands at  $207.9\text{ cm}^{-1}$  and  $755.8\text{ cm}^{-1}$  can be assigned to the surface intensified Raman vibration of polymer induced by  $\text{CrSi}_2$  nanocrystal.

Base on all the results discussed above, we conclude that  $\text{CrSi}_2$  nanocrystal can be well encapsulated with styrene/acrylonitrile copolymer. The encapsulation can not only improve the dispersed state of  $\text{CrSi}_2$  nanocrystal, maintain the properties of isolated particle, but also offer an effective way to its further assembly and manipulation. Such a study will also be beneficial to other semiconductor nanocrystals' system.

### Acknowledgement

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