Crystal structure analyses of ZnO nanoparticles growth by simple wet chemical method

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Crystal structure analyses of ZnO nanoparticles growth by simple wet chemical method

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Abstract. We have synthesized ZnO nanoparticles by using simple wet chemical method at calcination temperature of 400°C for 2 hours. Scanning electron microscopy (SEM) and X-ray diffraction (XRD) were performed to analyse morphology and crystal structure of ZnO nanoparticles, respectively. Morphologically, ZnO nanoparticles aggregated formed larger particles. Then, according to the International Center for Diffraction Data (ICDD) number #98-002-9272, the XRD spectra confirmed that the ZnO nanoparticles have polycrystalline hexagonal structure with prefer orientation of (002) and crystallite size in the range 21 nm.

1. Introduction
ZnO as II-VI semiconductor material with wide band gap energy of 3.34 eV and large exciton binding energy (60 mV) at room temperature is a potential material for optoelectronic applications [1,2]. In the last two decades, ZnO nanostructures have been studied theoretically and experimentally [3–5]. Scientists and engineers believed that the specific form ZnO nanostructure has a different application [3,6]. Compared with other nanostructures, ZnO nanoparticles with the range of 100 nm have a large specific surface area and small size effect [7]. Furthermore, ZnO nanoparticles have paid considerable attention due to quantum confinement effects which control optical properties of ZnO [7,8].

There are many methods to synthesize ZnO nanoparticles such as wet chemical [9], thermal decomposition, hydrolysis, hydrothermal, vapor transport, etc [10,11]. Among of these methods, wet chemical offers low-cost and has been used to synthesized different ZnO nanostructure [12].

In small concentrations, ZnO nanoparticles strongly inhibit the action of pathogenic microbes [13]. It also possesses antibacterial and antifungal activities [7]. Interestingly, ZnO nanoparticles have used to enhance electrochemiluminescence of luminol which used cancer biomarker detection [14]. Recently, ZnO nanoparticles are believed have a potential application as photocatalyst [11]. Even though, synthesized and characterization of ZnO nanoparticles still become major interest due to abundant their potential applications.

In this paper, we report structure analysis of ZnO nanoparticles which synthesized with simple wet chemical method. The morphology of powder ZnO nanoparticles have been observed by scanning electron microscopy (SEM) JEOL JSM-6510, X-ray diffraction (XRD) measurement with CuKα radiation (PAN-analytical), and compositions of precursors have been observed by energy dispersive X-ray.
2. Experimental
Zinc Chloride (ZnCl2) and Sodium Hydroxide (NaOH) were used as Zn precursor and for controlling pH in solution. Each of ZnCl2 and NaOH was dissolved in de-ionized (DI) water to obtained various molarities. The NaOH solution was added into ZnCl2 solution drop by drop under vigorous stirring without any heat treatment until a white suspension formed. ZnCl2 the molarities of ZnCl2/NaOH are 0.4/0.8 (ZnO-A), 0.4/0.4 (ZnO-B), and 0.8/0.4 (ZnO-C). Then, each of the suspension solutions was centrifuged to obtain precipitated of Zn(OH)2. Finally, the precipitation of Zn(OH)2 was calcined at the temperature of 400°C to obtain powder ZnO nanoparticles.

3. Results and discussion
Figure 1 (a)-(c) show SEM images of powder ZnO nanoparticles various compositions of ZnCl2/NaOH ratios. It can be observed that the ZnO nanoparticle aggregate tremendously. More clearly images of the aggregation can be confirmed in figure 1 (a). As seen from the figure 1(b) and (c), the aggregation of nanoparticles quite large. The aggregation of ZnO nanoparticles are predicted due to high surface energy of ZnO nanoparticles during calcination [15].

We further investigated the composition of powder ZnO particles by energy dispersive X-ray (EDAX). In can be seen from the table 1 that the ZnCl2/NaOH ratio of 0.4:0.8 yield the optimum composition ratio to synthesized ZnO nanoparticles.

![SEM images of powder ZnO nanoparticles various compositions of ZnCl2/NaOH ratios.](image)

The atomic percentage of Zn and O are 48.24% and 51.76%, respectively.
Table 1. Elements composition of ZnCl₂/NaOH ratio.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Precursor (Molaritas)</th>
<th>EDAX Analysis (At.%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ZnCl₂</td>
<td>NaOH</td>
</tr>
<tr>
<td>ZnO-A</td>
<td>0.4</td>
<td>0.8</td>
</tr>
<tr>
<td>ZnO-B</td>
<td>0.4</td>
<td>0.4</td>
</tr>
<tr>
<td>ZnO-C</td>
<td>0.8</td>
<td>0.4</td>
</tr>
</tbody>
</table>

Figure 2 show XRD pattern of ZnO nanoparticles with various compositions of ZnCl₂/NaOH ratios. According to the XRD pattern, we confirm that the sample ZnO-A with ZnCl₂/NaOH ratio of 0.4:0.8 have only one phase ZnO. Meanwhile, ZnO-B and ZnO-C have other phases such as Zn(OH)₂.

According the XRD pattern of ZnO-A as shown in fig. 2, we observed eleven peaks with the hkl are (100), (002), (101), (102), (110), (103), (200), (112), (201), (004), and (202). Among of these peaks, the peaks belongs to hkl (100), (002), and (101) are more intense compared with others.

![XRD pattern](image)

Figure 2. XRD pattern of ZnO nanoparticles with various compositions of ZnCl₂/NaOH ratios.

Refer to the International Center for Diffraction Data (ICDD) number #98-002-9272, the powder ZnO nanoparticles have a hexagonal wurtzite structure.

Table 2. The data of full width at half maximum (FWHM), crystallite size, and lattice strain of ZnO nanoparticle structure at hkl of (002).

<table>
<thead>
<tr>
<th>No.</th>
<th>2 theta</th>
<th>hkl</th>
<th>FWHM</th>
<th>Crystallite size (nm)</th>
<th>Lattice Strain (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>31.837</td>
<td>100</td>
<td>0.307</td>
<td>21.872</td>
<td>0.650</td>
</tr>
<tr>
<td>2</td>
<td>34.502</td>
<td>002</td>
<td>0.316</td>
<td>21.586</td>
<td>0.600</td>
</tr>
<tr>
<td>3</td>
<td>36.334</td>
<td>101</td>
<td>0.322</td>
<td>21.342</td>
<td>0.580</td>
</tr>
</tbody>
</table>
References

Financial support from the National Science and Engineering Research Council of Canada (NSERC) is gratefully acknowledged.

4 Conclusions

Figure 3. Coefficient of linear extension of ZnO nanowires with ZnCl\(_2\)/NH\(_4\)Cl ratios of 0.8.

In order to confirm the published equation, we calculated quadratically coefficient of linear by using this equation (18).

\[ \frac{I_{(002)}/I_{(101)}}{I_{(002)}/I_{(101)}} = \frac{\beta_{(002)}}{\beta_{(101)}} \]

The ratio of (002) is greater than (101). Figure 1 shows a quadratic regression analysis and is the real number of reflection peaks for the sample. In the plane (hkl) is that from the XRD pattern of ZnO nanowires, it can be confirmed that the ratio of (002) is greater than (101).
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