Anisotropy of Zn Structure Semiconductors

Faeq A. A. Radwan
Faculty of Engineering, Near East University, K. K. T. C. Lefkosa
P.O. Box: 670, Mersin - 10, Turkey

Abstract: The norm of elastic constant tensor and the norms of the irreducible parts of the elastic constants of Zn structure semiconductors are calculated. The relation of the scalar parts norm and the other parts norms and the anisotropy of the material are presented. The norm ratios are used as a criterion to present the anisotropy degree of the properties of the material. The ratio \( \frac{N}{C_0} \) is calculated, where \( N \) is the norm of elastic constant tensor of the material, and \( C_0 \) is the elastic constant of the crystal in the order of magnitude \( e^2 / r^4 \), where \( e \) is the charge of the electron, and \( r \) is the distance between the nearest neighbor atom. Also the comparison of \( \frac{N}{C_0} \) with Zinc Blende lattice parameter, Zinc Blende density, and Energy Gap at 300 K are given in (Radwan, 2001).

Key Words: Norm, Anisotropy, Elastic Constant, Irreducible, and Nearest Neighbor Atom

Introduction
Group II-VI Compound Semiconductors (Zn Structure Semiconductors) Materials can crystallize in either the cubic zinc Blende ( sphalerite) phase, or the hexagonal wurzite phase. The decomposition of the elastic constant tensor to its irreducible parts and the norm concept and its relation to anisotropy are given in (Radwan, 2001). Group II-VI Compound Semiconductors: The elastic constants of II-VI Compound Semiconductors are given in the following Table, (Landolt-Bornstein, Group III).

Table 1: Elastic constants in \( 10^{11} \text{ dyn/cm}^2 \)

<table>
<thead>
<tr>
<th>Material</th>
<th>( C_{11} )</th>
<th>( C_{12} )</th>
<th>( C_{44} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group II-VI</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ZnS</td>
<td>10.40</td>
<td>6.50</td>
<td>4.62</td>
</tr>
<tr>
<td>Semiconductors</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ZnSe</td>
<td>8.10</td>
<td>4.88</td>
<td>4.41</td>
</tr>
<tr>
<td>ZnTe</td>
<td>7.13</td>
<td>4.07</td>
<td>3.12</td>
</tr>
<tr>
<td>CdS</td>
<td>7.79</td>
<td>5.27</td>
<td>2.41</td>
</tr>
<tr>
<td>CdSe</td>
<td>6.67</td>
<td>4.63</td>
<td>2.23</td>
</tr>
<tr>
<td>CdTe</td>
<td>5.35</td>
<td>3.68</td>
<td>1.99</td>
</tr>
<tr>
<td>HgS</td>
<td>8.13</td>
<td>6.22</td>
<td>2.64</td>
</tr>
<tr>
<td>HgSe</td>
<td>6.03</td>
<td>4.39</td>
<td>2.22</td>
</tr>
<tr>
<td>HgTe</td>
<td>5.32</td>
<td>3.68</td>
<td>2.08</td>
</tr>
</tbody>
</table>

By using Table 1, the decomposition of the elastic constant tensor and the norm concept we can calculate the norms and the norm ratios of the given materials as in the following Table.
Table 2: The norms and norm ratios (the anisotropy degree)

<table>
<thead>
<tr>
<th>Material</th>
<th>$N_s$</th>
<th>$N_n$</th>
<th>$N$</th>
<th>$N_s/N$</th>
<th>$N_n/N$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CdS</td>
<td>19.4375</td>
<td>2.107985</td>
<td>19.55147</td>
<td>0.994171</td>
<td>0.107817</td>
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<tr>
<td>CdSe</td>
<td>16.94988</td>
<td>2.217967</td>
<td>17.09438</td>
<td>0.991547</td>
<td>0.129748</td>
</tr>
<tr>
<td>HgS</td>
<td>21.57873</td>
<td>3.088656</td>
<td>21.79866</td>
<td>0.989911</td>
<td>0.14169</td>
</tr>
<tr>
<td>CdTe</td>
<td>13.68308</td>
<td>2.11715</td>
<td>13.8459</td>
<td>0.98824</td>
<td>0.152908</td>
</tr>
<tr>
<td>ZnTe</td>
<td>17.35067</td>
<td>2.914518</td>
<td>17.59375</td>
<td>0.986184</td>
<td>0.165656</td>
</tr>
<tr>
<td>HgTe</td>
<td>13.71510</td>
<td>2.309618</td>
<td>13.90821</td>
<td>0.986115</td>
<td>0.166062</td>
</tr>
<tr>
<td>ZnS</td>
<td>26.19816</td>
<td>4.894191</td>
<td>26.65139</td>
<td>0.982994</td>
<td>0.183637</td>
</tr>
<tr>
<td>ZnSe</td>
<td>20.92952</td>
<td>5.132485</td>
<td>21.54964</td>
<td>0.971223</td>
<td>0.23817</td>
</tr>
<tr>
<td>HgSe</td>
<td>17.772</td>
<td>6.543918</td>
<td>18.9385</td>
<td>0.938406</td>
<td>0.345535</td>
</tr>
</tbody>
</table>

Table 3: Calculated values of $(N_s, r^2, C_0, N / C_0)$ (Landolt-Börnstein Group III and Palmer, 2000.08)

<table>
<thead>
<tr>
<th>Material</th>
<th>$r \times 10^{-8}$ cm$^2$</th>
<th>$r^4 \times 10^{-31}$</th>
<th>$\epsilon \times 10^{-10}$</th>
<th>$e^2 \times 10^{-19}$</th>
<th>$C_0 = e^2 / r^4 \times 10^{11}$</th>
<th>$N \times 10^{12}$</th>
<th>$N / C_0$</th>
<th>Zinc Blende Lattice Parameter at 300K</th>
<th>$g.cm^{-3}$ 300K</th>
<th>Energy Gap $E_g$ at 300K</th>
</tr>
</thead>
<tbody>
<tr>
<td>HgSe</td>
<td>2.64</td>
<td>4.86</td>
<td>4.80</td>
<td>2.30</td>
<td>4.74</td>
<td>1.89</td>
<td>3.98</td>
<td>6.09</td>
<td>8.22</td>
<td>...</td>
</tr>
<tr>
<td>HgS</td>
<td>2.53</td>
<td>4.10</td>
<td>4.80</td>
<td>2.30</td>
<td>5.62</td>
<td>2.18</td>
<td>3.88</td>
<td>5.85</td>
<td>4.72</td>
<td>...</td>
</tr>
<tr>
<td>CdTe</td>
<td>2.81</td>
<td>6.21</td>
<td>4.80</td>
<td>2.30</td>
<td>3.71</td>
<td>1.38</td>
<td>3.73</td>
<td>6.48</td>
<td>5.86</td>
<td>1.475</td>
</tr>
<tr>
<td>CdSe</td>
<td>2.63</td>
<td>4.78</td>
<td>4.80</td>
<td>2.30</td>
<td>4.82</td>
<td>1.79</td>
<td>3.72</td>
<td>6.08</td>
<td>5.65</td>
<td>1.751</td>
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<tr>
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<td>2.64</td>
<td>4.84</td>
<td>4.80</td>
<td>2.30</td>
<td>4.76</td>
<td>1.76</td>
<td>3.70</td>
<td>6.10</td>
<td>5.65</td>
<td>2.394</td>
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<tr>
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<td>2.79</td>
<td>6.06</td>
<td>4.80</td>
<td>2.30</td>
<td>3.80</td>
<td>1.39</td>
<td>3.66</td>
<td>6.45</td>
<td>8.12</td>
<td>...</td>
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<tr>
<td>ZnS</td>
<td>2.34</td>
<td>3.01</td>
<td>4.80</td>
<td>2.30</td>
<td>7.65</td>
<td>2.67</td>
<td>3.48</td>
<td>5.41</td>
<td>4.11</td>
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<td>2.52</td>
<td>4.03</td>
<td>4.80</td>
<td>2.30</td>
<td>5.71</td>
<td>1.96</td>
<td>3.43</td>
<td>5.82</td>
<td>4.87</td>
<td>2.50</td>
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<tr>
<td>ZnSe</td>
<td>2.45</td>
<td>3.63</td>
<td>4.80</td>
<td>2.30</td>
<td>6.34</td>
<td>2.15</td>
<td>3.40</td>
<td>5.67</td>
<td>5.26</td>
<td>2.8215</td>
</tr>
</tbody>
</table>

**Conclusion**

From Table (2) we can conclude that CdS (Cadmium Sulfide) is the most isotropic material with the highest value of $N_s/N$ and the lowest value of $N_n/N$, and HgSe (Mercury Selenide) is the most anisotropic material with the highest value of $N_n/N$ and with the lowest value of $N_s/N$, because for isotropic material $N_s/N = 1$ and $N_n/N = 0$. Which means that as $N_s/N$ increases the anisotropy increases. And also the most strong material is ZnS (Zinc Sulfide) which has the highest value of $N$ with the highest Energy Gap, 3.68 eV (Table (3)).

From Table (3) we can see that the range of $\frac{N}{C_0}$ varies from 3.98 for HgSe (Mercury Selenide) with the highest density to 3.40 for ZnSe (Zinc Selenide) for II-VI semiconductors.

**References**

D. W. Palmer, 2000.08. 'Major Properties of the II-VI Compound Semiconductors' www.semiconductors.co.uk