ANALYSIS OF TEMPERATURE DEPENDENCE OF ANDERSON-GRUNEISEN PARAMETER FOR ZnO NANORODS

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ABSTRACT

In the present manuscript, the theoretical results on temperature dependence of Anderson-Gruneisen parameter for zinc oxide (ZnO) nanorods have been reported. For the purpose, Anderson-Gruneisen parameter equation has been used. Considering bulk modulus and volume thermal expansivity, Anderson-Gruneisen parameters for zinc oxide (ZnO) nanorods (rock salt phase and wurtzite phase) have been calculated in the temperature range starting from room temperature upto melting point. It is found that Anderson-Gruneisen parameter increases sharply in the temperature range starting from room temperature 300 K upto melting point 2248 K for both the phases of zinc oxide (ZnO) but the rate of increase is higher in the case of rs-ZnO in comparision of wurtzite phase of ZnO.

KEYWORDS: Anderson-Gruneisen Parameter, Zinc Oxide, Nanorods

INTRODUCTION

The nanomaterials are expected to be the turning point of the next technological revolution in solid state electronics and to have a considerable impact practically in all domains of science. Recently, zinc oxide (ZnO) has attracted much attention within the scientific community as a ‘future material’. This is however, somewhat of a misnomer, as ZnO has been widely studied since 1935[C.W. Bunn, 1935], with much of our current industry and day-to-day lives critically reliant upon this compound.

The renewed interest in this material has arisen out of the development of growth technologies for the fabrication of high quality single crystals and epitaxial layers, allowing for the realization of ZnO-based electronic and optoelectronic devices.

Zinc oxide (ZnO) belongs to the family of wide-band-gap semiconductors with strong ionic character of chemical bonds. At ambient conditions ZnO has wurtzite structure (P63mc, w-ZnO) that transforms into rock-salt one (Fm3m, rs-ZnO) at pressures above 5 GPa [K.Kusaba et al, 1999; V.L. Solozhenko et al, 2011]. Upon pressure release rs-ZnO reverts back to wurtzite phase[F. Decremps et al, 2003]. Recently, it has been shown that nanocrystalline rs-ZnO synthesized at high pressures and high temperatures can be completely recovered at normal conditions[V.L. Solozhenko et al, 2011]

Some workers have worked on temperature dependence of Anderson-Gruneiesen parameter for various solids[K.Y. Singh et al, 2003; R.S. Chauhan et al, 2007; Chunhui Nie et al, 2010] and have employed various approaches for the determination of Anderson-Gruneisen parameter. However, the study of temperature dependence of Anderson-Gruneisen parameter for ZnO nanorods is still lacking. Therefore, it is planned to analyze the temperature dependence of Anderson-Gruneisen parameter for zinc oxide (ZnO) nanorods which is very important from scientific and industrial point of view. The method of analysis of temperature dependence of Anderson-Gruneisen parameter for zinc oxide (ZnO) nanorods is given in section 2 and results and discussion are given in section 3.
METHOD OF ANALYSIS

Anderson-Gruniesen parameter ($\delta_T$) is defined as [O.L. Anderson et al, 1992]-

$$\delta_T = \frac{1}{\alpha_T} \left( \frac{\delta K_T}{\delta T} \right)$$

where $\alpha$ is volume thermal expansivity, $K_T$ isothermal bulk modulus.

The following relationships have been presented [K.S. Singh et al, 2002]-

$$\alpha = a_0 [1 + 1.35 a_0 \delta_T^0 (T - T_0)]$$

$$K_T = K_0 [1 - 1.06 a_0 \delta_T^0 (T - T_0)]$$

Where $a_0$ is volume thermal expansivity at room temperature, $\delta_T^0$ Anderson-Gruniesen parameter at room temperature ($T_0$), $K_0$ bulk modulus at room temperature.

Substituting equations (2) and (3) in equation (1), the expression for Anderson-Gruniesen parameter is obtained as follows-

$$\delta_T = \frac{1.06 \delta_T^0}{[1 + 1.35 a_0 \delta_T^0 (T - T_0)][1 - 1.06 a_0 \delta_T^0 (T - T_0)]}$$

The following expressions for temperature dependence of $\frac{V}{V_0}$ and the isothermal bulk modulus $K_T$ have been obtained [Z.H. Fang, 2005]-

$$\frac{V}{V_0} = 1 - \delta_T^0 \ln[1 - a_0 \delta_T^0 (T - T_0)]$$

$$K_T = K_0 [1 - a_0 \delta_T^0 (T - T_0)]$$

where $V_0$ is the initial volume and $V$ final volume. Thus Anderson-Gruniesen parameter has been expressed as-

$$\delta_T = \frac{1.06 \delta_T^0}{[1 + 1.35 a_0 \delta_T^0 (T - T_0)][1 - 1.06 a_0 \delta_T^0 (T - T_0)]}$$

Using equation (7), the temperature dependence of Anderson-Gruniesen parameter for ZnO rock salt phase and ZnO wurtzite phase has been analysed.

RESULTS AND DISCUSSIONS

Equation (7) represents the temperature dependence of Anderson-Gruniesen parameter ($\delta_T$). The input parameters used in the present work have been shown in Table 1. The theoretical values of $\delta_T$ have been calculated in the temperature range starting from room temperature 300 K upto the melting point 2248 K for both phases of zinc oxide (ZnO) i.e. ZnO rock salt phase and ZnO wurtzite phase. Figure (1) shows the variation of $\delta_T$ with temperature for both phases of zinc oxide (ZnO). Figure 1(a) represents the variation of $\delta_T$ with temperature for rs-ZnO while figure 1(b) shows the variation of $\delta_T$ with temperature for wurtzite phase.

From figure (1) it is clear that $\delta_T$ increases with temperature with constant rate for both ZnO- rocksalt phase and ZnO- wurtzite phase but this rate of increase is more in case of rs-ZnO. The experimental observations on temperature dependence of $\delta_T$ for ZnO are not appearing in the literature. However, this variation of $\delta_T$ with temperature is similar as in the case of other solids [Chuanhui Nie et al, 2010]. It is concluded that Anderson-Gruniesen parameter ($\delta_T$) increases...
Analysis of Temperature Dependence of Anderson-Gruneisen Parameter or ZnO Nanorods

A sharply in the temperature range starting from room temperature 300 K up to melting point 2248 K for both the phases of ZnO but the rate of increase is higher in the case of rs-ZnO i.e. in the case of rock salt phase of ZnO the Anderson-Gruneisen parameter ($\delta_T$) is more sensitive with temperature as in the comparison of wurtzite phase of ZnO phase.

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REFERENCES


APPENDICES

Table 1: Input Parameters Used in the Present Work

<table>
<thead>
<tr>
<th>Material</th>
<th>Bulk Modulus at Room Temperature $K_0$(GPa)</th>
<th>Volume Thermal Expansivity at Room Temperature $\alpha_0$ (K$^{-1}$)</th>
<th>Anderson-Gruneisen Parameter at Room Temperature $\delta_T$</th>
<th>Melting Point (K)</th>
</tr>
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</table>
Figure 1: Variation of Anderson-Gruneisen Parameter ($\tilde{\gamma}$) with Temperature (T) for (a) Rock Salt Phase of ZnO: Solid Triangle (b) Wurtzite Phase of ZnO: Solid Square