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# Mechanical, elastic and anharmonic properties of $Zn_{1-x}Cr_xTe(0\leq x\leq 1)$ diluted magnetic semiconductor

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The mechanical, elastic and anharmonic properties of II –VI diluted magnetic semiconductor $Zn_{1-x}Cr_xTe$ ($0\leq x\leq 1$) have been reported by using a phenomenological model based on the charge transfer effects due to the deformation of the electronic shell of overlapping ions. The obtained results on the elastic properties agree reasonably well with the available experimental data. The Debye temperature, third order elastic constants and the pressure derivatives of second order elastic constants have also been reported. The decrease in Debye temperature with the increase in Cr concentration suggests that the lattice gets soften with the increase of Cr concentration.

**Keywords**: Magnetic semiconductor, Charge transfer, Elastic constants

**IPC Code:** H01L

## 1 Introduction

Diluted magnetic semiconductors (DMS's), due to their unique characteristics have become important materials in the field of opto-electronic devices such as solar cells, IR detectors, magnetic field sensors and optical isolators[1]. Recently, many investigations are focused on the application of the concept of spintronics or magneto electronics in DMS's, because they provide testing ground for spintronics due to their simple band structures and excellent magneto optical and transport properties[2].

Group III-V and II-VI ferromagnetic diluted magnetic semiconductors are important materials for the applications of spintronics due to their good compatibilities with existing semiconductor devices[3]. It is observed that the ferromagnetic long range ordering in Mn-doped III-V DMS's such as $Ga_{1-x}Mn_xAs$ and $In_{1-x}Mn_xAs$ are caused by the carrier mediated ferromagnetic interaction between the localized *d* spins of Mn ions[4]. The $Mn^{+2}$ ion doped DMS's $Ga_{1-x}Mn_xAs$ have highest Curie temperature as high as 110 K (Ref. 4). Recently, ferromagnetic II-VI DMS's have also been observed in heavily *p*-doped $Zn_{1-x}Cr_xTe$ and $Be_{1-x}Mn_xTe$, but with lower *T*c (~2-3 K) (Ref. 5). The doping inevitably changes both conductive and optical properties, and to control both independently it is desired to obtain ferromagnetic DMS. Thus, ferromagnetic II-VI DMS's are very promising materials for device applications.

Cr doped DMS's are crucial due to their *d-d* super exchange interaction which predicts ferromagnetism within it[6]. Satio *et al*.[7] and Okazawa *et al.*[8] observed this ferromagnetic *d–d* exchange in $Ga_{1-x}Cr_xAs$ epitaxial films. It has been theoretically proved that this ferromagnetic state is more stable than that in nonmagnetic state in Cr doped II-VI DMS (Ref. 9). An exchange interaction between *p*-holes and *d* spin of Cr ions has been reported in Cr doped II-VI DMS's such as $Zn_{1-x}Cr_xTe$ (Ref.10). Recently, Saito *et al*.[11] have reported a ferromagnetic hysteresis loop in magnetization curve of an epitaxial film of $Zn_{1-x}Cr_xTe$ ($x$=0.035) (Ref. 11) and a quite high transition temperature [12] of around 300 K. Looking to the importance of Cr doped ZnTe II-VI DMS's, it is a right juncture to investigate the physical properties of this compound.

There are number of crucial investigations on ferromagnetic II-VI $Zn_{1-x}Cr_xTe$ but up to the best of our knowledge, the detailed study of mechanical, elastic and anharmonic properties for this material is yet to come. These properties are not only important as fundamental properties of the considered diluted magnetic semiconductor, but are also to understand if the changes in elastic or mechanical properties influence the structural stability. If there is reduction in the elastic constants with the concentration that may lead to structural instability due to hybridization of Mn and Te orbital for tetrahedral bond formation

and finally for the larger anion-mediated super-exchange in ZnCrTe diluted magnetic semiconductor compounds.

Motivated by this fact we have investigated the mechanical, elastic and anharmonic properties of $Zn_{1-x}Cr_xTe$ for the first time by using a simple potential approach. This investigation includes a description of the second order elastic constants (SOEC), bulk modulus, shear modulus, anisotropy, third order elastic constants (TOEC), pressure derivatives of SOEC, thermal properties such as Debye temperature by using a inter-atomic potential under the frame work of three-body potential approach[13]. This three-body interaction arises due to the effect of charge transfer from the deformation of electron shells due to the overlap of neighbouring ions[14,15]. This effect has been introduced phenomenologically in the potential and considered as a model parameter. This approach has been quite successful in explaining the static, dynamical and structural properties of several compounds including diluted magnetic semiconductors[12-16].

## 2 Theoretical Description

The formula for three body interaction potential under the frame work of three body interaction approach is taken from singh & Singh[14] and Rao & Sanyal[15] and is expressed as,

$$U(r) = \sum_{i,j}{}' \frac{z_i z_j e^2}{r_{ij}} + \sum_{i,j,k}{}' \frac{z_i z_j e^2 f(r_{ik})}{r_{ij}} + \sum_{i,j}{}' b\beta_{ij} \exp\left[\frac{(r_i + r_j - r_{ij})}{\rho_{ij}}\right] \quad \ldots (1)$$

where, first term represents long range columbic interaction, second term represents three body interaction arising from charge transfer effects and final term represents HF form of short range repulsive energies. Equation (1) consists of three parameters: Hardness parameter *b*, strength parameter ρ and TBI parameter *f*(r), where *f*(r) = $f_{0*}\exp(-r_{ij}/\rho)$ and is considered to be effective up to first neighbour only. For the simplicity only single ρ has been used. While the hardness and strength parameter *b* and ρ are obtained from the equation for bulk modulus and equilibrium conditions[16-17], the TBI parameter *f*(r) is obtained from overlap integrals[15]. The higher order derivative of *f*(r) can be evaluated by assuming the above function form. βij is Pauling constant and can be expressed as βij = 1+ $(Z_i/n_i)+(Z_j/n_j)$ with $Z_i(Z_j)$ and $n_i$ $(n_j)$ as the valency and number of outermost electrons in the anions (cations), respectively. The values of input parameters and obtained model parameters for $Zn_{1-x}Cr_xTe$ ($0 \le x \le 1$) are shown in Table 1 using inter atomic potential given in Eq. (1) the expressions for SOEC.

## 3 Results and Discussion

For the first time, an investigation of mechanical, elastic and anharmonic properties of ferromagnetic $Zn_{1-x}Cr_xTe$ for concentration $0 \le x \le 1$ has been carried out. This includes second order elastic constants (SOEC), third order elastic constants (TOEC), pressure derivatives, Debye temperature, specific heat, anisotropy, shear modulus etc. by using a theoretical model discussed in Sec. 2. The second order elastic constants $C_{11}$, $C_{12}$ and $C_{44}$ have been obtained by using expressions derived from Eq. (1) and found in Ref. 16. The SOEC obtained so, have been presented in Table 2. The results obtained on the elastic constants from the present approach are in good agreement with the available experimental

Table 1— Input data and model parameter for $Zn_{1-x}Cr_xTe$ ($0 \le x \le 1$)

| Concentration | Input parameter | | | | Model Parameter | | | |
|---|---|---|---|---|---|---|---|---|
| | $r_+$ (A°) | $r_-$ (A°) | r (A°) | $B_T$ ($10^{11}$ dyne/cm$^2$) | a (A°) | *b* ($10^{-19}$ J) | ρ (A°) | *f*(r) |
| ZnTe | 0.74 | 2.11 | 3.050 | 5.28[a]<br>5.28[b]<br>5.08[c] | 6.100<br>6.100[a] | 2.713 | 0.41 | -0.07318 |
| $Zn_{0.8}Cr_{0.2}Te$ | 0.77 | 2.11 | 3.069 | 5.14 | 6.138 | 2.619 | 0.413 | -0.07310 |
| $Zn_{0.6}Cr_{0.4}Te$ | 0.80 | 2.11 | 3.088 | 5.00 | 6.176 | 2.472 | 0.422 | -0.07190 |
| $Zn_{0.4}Cr_{0.6}Te$ | 0.83 | 2.11 | 3.107 | 4.86 | 6.215 | 2.451 | 0.424 | -0.07285 |
| $Zn_{0.2}Cr_{0.8}Te$ | 0.86 | 2.11 | 3.127 | 4.70 | 6.254 | 2.382 | 0.426 | -0.07243 |
| CrTe | 0.89 | 2.11 | 3.146 | 4.59[a]<br>4.59[d] | 6.292[a]<br>6.29[d] | 2.299 | 0.428 | -0.07248 |

[a] From our present calculation
[b] From Ref. 16.
[c] From Ref. 17.
[d] From Ref. 18.

data[18,19]. Table 2 reveals that there is a slight underestimation of the value of elastic constant $C_{44}$ for ZnTe in comparison to experimentally obtained value. It can be inferred from Table 2 that the difference between the results on the $C_{44}$ between present calculation and *ab-initio* calculation increases for CrTe. But looking to the trend of elastic constants $C_{44}$ with the concentration of *x* and the experimental value ZnTe, it seems that the value obtained from *ab-initio* calculations is overestimated. To have an exact order of the elastic constants, the elastic constants of Mn doped CdTe diluted magnetic semiconductor[13] (DMS) has also been presented in Table 2. The elastic constants can be used to calculate the anisotropy factor and shear modulus of a compound to understand whether the medium is isotropic or not. If anisotropy factor $A$ =1 for any material, its elastic properties are close to the isotropic medium and the value of $A$ less than 1, the material will show considerable anisotropy in medium. The obtained results of elastic constants are used to calculate the value of anisotropy factor $A$ and shear modulus $S$ by using following relations[20] and presented in Table 2.

$$A= C_{11}-C_{12}/ 2\ C_{44} \text{ and } S= C_{11}-C_{12}/2 \quad \ldots (2)$$

The value of anisotropy factor is about 0.62 for these compounds shows that these compounds are having anisotropy in their elastic properties. The Debye temperature of a compound gives the idea of stiffness of material. The decrease in $\theta_D$ with increase in Cr concentration points to the softening of lattice. This can be understood from the fact that the increase in Cr concentration increases the lattice parameters. We have also calculated the Debye temperature for $Zn_{1-x}Cr_xTe$ for different concentration of Cr using the following expression[21]:

$$\theta_D = C_B\ (a\ G_B/M)^{1/2}$$
$$\text{where } G_B = [C_{44}(C_{11}-C_{12})(C_{11}+C_{12}+2C_{44})]^{1/3} \quad \ldots (3)$$

where $a$ is a lattice constant $M$, the atomic weight , $C_B = 3.89 \times 10^{11} \times S^{-1/6}\ h/K_B$ with $h$ as Planck's constant, and $K_B$, the Boltzmann constant and $S$ the number of atoms per unit cell. The value of Debye temperature presented in Table 3, could not be compared for all values of $x$ (Cr concentration). However, the value of Debye temperature obtained for ZnTe by using the present simple approach is, in general, good agreement with the available data. It can be seen from the table that the values of Debye temperature obtained for the different values of $x$ are very close to the Debye temperature value of ZnTe and not much variation is observed. However, Table 3 depicts the decrease in the Debye temperature of these compounds with the increase of Cr concentration, which implies that the lattice is getting softened with the increase of Cr concentration. This can be in fact supported by the fact that the lattice parameters of Cr doped ZnTe increases with the increase of Cr. As far as the success of the approach in predicting the Debye temperature is concerned, we cannot make any

Table 2— Second order elastic constants, Anisotropy factor and Shear modulus for zinc blende $Zn_{1-x}Cr_xTe$ ($0 \le x \le 1$)

| Concentration | Elastic constants ($10^{11}$dyne/cm$^2$) | | | Anisotropy Factor $A$ | Shear modulus $S$ ($10^{11}$dyne/cm$^2$) |
|---|---|---|---|---|---|
| | $C_{11}$ | $C_{12}$ | $C_{44}$ | | |
| | 7.321[a] | 4.259[a] | 2.404[a] | | |
| ZnTe | 7.110[b] | 4.070[b] | 3.130[b] | 0.6367 | 0.1530 |
| | 7.110[c] | 4.070[c] | 3.130[c] | | |
| $Zn_{0.8}Cr_{0.2}Te$ | 7.131 | 4.145 | 2.343 | 0.6371 | 0.1493 |
| $Zn_{0.6}Cr_{0.4}Te$ | 6.975 | 4.015 | 2.337 | 0.6331 | 0.1480 |
| $Zn_{0.4}Cr_{0.6}Te$ | 6.753 | 3.977 | 2.227 | 0.6231 | 0.1388 |
| $Zn_{0.2}Cr_{0.8}Te$ | 6.538 | 3.781 | 2.172 | 0.6344 | 0.1378 |
| CrTe | 6.386 | 3.691 | 2.118[a] | 0.6359 | 0.1347 |
| | | | 3.64[d] | | |
| $Cd_{0.94}Mn_{0.96}Te$[e] | 5.3 | 3.7 | 1.99 | - | - |
| $Cd_{0.55}Mn_{0.45}Te$[e] | 5.1 | 3.5 | 1.84 | | |
| $Cd_{0.48}Mn_{0.52}Te$[e] | 5.1 | 3.5 | 1.82 | | |
| $Cd_{0.52}Mn_{0.18}Te$[e] | 6.0 | 3.8 | 4.50 | | |

[a] From our present calculation
[b] From Ref. 16.
[c] From Ref. 17.
[d] From Ref. 18.
[e] From Ref. 13.

Table 3— Debye temperature, third order elastic constants ($\times 10^{11}$ dyne/cm$^2$) and pressure derivatives of $Zn_{1-x}Cr_xTe$ ($0 \le x \le 1$)

| Parameter | ZnTe | $Zn_{0.8}Cr_{0.2}Te$ | $Zn_{0.6}Cr_{0.4}Te$ | $Zn_{0.4}Cr_{0.6}Te$ | $Zn_{0.2}Cr_{0.8}Te$ | CrTe |
|---|---|---|---|---|---|---|
| $\theta_D$ (K) | 185.27[a]<br>180±6[b]<br>225.3[c] | 184.77 | 185.718 | 183.22 | 183.058 | 182.78 |
| $C_{111}$ | -20.26 | -19.70 | -18.59 | -18.52 | -17.69 | -17.33 |
| $C_{112}$ | -25.18 | -24.50 | -23.45 | -23.19 | -22.82 | -21.7 |
| $C_{123}$ | -14.90 | -14.46 | -13.32 | -13.52 | -12.82 | -12.56 |
| $C_{144}$ | 0.704 | 0.710 | 1.101 | 0.753 | 0.865 | 0.828 |
| $C_{166}$ | -13.04 | -12.69 | -12.32 | -12.00 | -11.58 | -11.32 |
| $C_{456}$ | 6.607 | 6.449 | 6.515 | 6.147 | 6.020 | 5.873 |
| dB/dP | 2.5048[a]<br>5.04[c] | 2.5004 | 2.4088 | 2.4818 | 2.4472 | 2.4541 |
| dS/dP | -0.589 | -0.5892 | -0.5797 | -0.5872 | -0.5837 | -0.584 |
| $dC_{44}/dP$ | 0.6757[a]<br>0.45[c] | 0.6734 | 0.6247 | 0.6635 | 0.6452 | 0.6488 |

[a] From our present calculation
[b] From Ref. 16.
[c] From Ref. 17.

comment at this stage but will emphasize for the specific heat measurement or the determination of the elastic constants for these compounds.

We have also calculated the anharmonic properties such as TOEC and Pressure derivatives of SOEC i.e. d*B*/d*P*, d*S*/d*P* and $dC_{44}/dP$ for $Zn_{1-x}Cr_xTe$ using the expressions presented elsewhere[13]. These results could not be compared with the experimental data due to unavailability. The calculated third order elastic constants and the pressure derivatives of elastic constants are listed in Table 3.

## 4 Conclusion

In the present paper, we have investigated mechanical elastic and anharmonic properties of $Zn_{1-x}Cr_xTe$ ($0 \le x \le 1$). Obtained results agree fairly well with the experimental data wherever they are available. Debye temperature decreases with increase in concentration of Cr at room temperature. Obtained value of anisotropy predicts that material will be anisotropic in elastic behaviour. The decrease of Debye temperature with the Cr concentration suggests that these compounds get softened with the increase of Cr concentration. Overall results are in good agreement with experimental values, which indicates success of our approach.

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