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A study on strain affecting electronic structures and optical properties of wurtzite $Mg_{0.25}$ $Zn_{0.75}O$ by first-principles*

Shi Li-Bin(史力斌)[a)†], Li Ming-Biao(李明标)[a)], Ren Jun-Yuan(任骏原)[a)], Wang Li-Jin(王立锦)[b)], and Xu Cui-Yan(徐翠艳)[c)]

[a)] *Department of Physics, Bohai University, Jinzhou* 121013, *China*
[b)] *School of Material Science and Engineering, University of Science and Technology Beijing, Beijing* 100083, *China*
[c)] *Department of Mathematics and Physics, Liaoning University of Technology, Jinzhou* 121000, *China*

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We have made a first principles study to investigate density of states, band structure, the dielectric function and absorption spectra of wurtzite $Mg_{0.25}Zn_{0.75}O$. The calculation is carried out in *a*-axis and *c*-axis strain changing in the range from 0.3 to –0.2 in intervals of 0.1. The results calculated from density of states show that the bottom of conduction band is always dominated by Zn 4s and the top of valence band is always dominated by O 2p in *a*-axis and *c*-axis strain. Zn 4s will shift to higher energy range when *a*-axis strain changes in the range from 0.3 to 0, and then shift to lower energy range when *a*-axis strain changes in the range from 0 to –0.2. But Zn 4s will always shift to higher energy range when *c*-axis strain changes in the range from 0.3 to –0.2. The variations of band gap calculated from band structure and absorption spectra are also investigated, which are consistent with the results obtained from density of states. In addition, we analyse and discuss the imaginary part of the dielectric function ε_2.

Keywords: first principles, density of states, band structure, dielectric function
PACC: 7000, 7115M, 7125

1. Introduction

Because ZnO has a wide band gap of 3.37 eV, high structure stability and large exciton binding energy of 60 meV at room temperature, it has been considered as a promising material in the field of ultraviolet light emitting devices and laser diodes.[1,2] A crucial step in designing modern optoelectronic devices is the realization of band gap engineering to create barrier layers and quantum wells. At present, two main problems present themselves. One is the realization of stable p-type conduction.[3] The pure ZnO generally shows n-type conduction due to the existence of oxygen vacancy and zinc interstitial. It is well known that the most suitable dopants for p-type ZnO are the group-V elements (N, P, As and Sb) to substitute for O. However it is very difficult to obtain p-type ZnO due to low solubility of the acceptor dopants, deep acceptor level and its self-compensating effect between the acceptor dopants and the intrinsic donors. Now, the codoping method is also presented in order to obtain stable p-type conduction,[4,5] which becomes a promising way to apply the material. Another problem that faces us is the modulation of band gap for ZnO.[6] The band gap for ZnO can be tuned by bivalent metals such as Cd and Mg substitution for Zn. CdO is a semiconductor with a direct band gap of 2.30 eV and MgO has a wider band gap of 7.83 eV. CaO and MgO are good solid solution with ZnO. It is found that $Mg_xZn_{1-x}O$ alloys have an adjustable band gap in the range from 3.37 to 7.83 eV,[7] and $Cd_xZn_{1-x}O$ alloys have an adjustable band gap in the range from 2.84 to 3.20 eV.[8] They have been already investigated extensively due to their potential applications.[9–14]

The thin films deposited on the substrates will show strain due to mismatch of crystal lattice. Strain in thin films has effect on electronic structures and optical properties, which offers an opportunity to enhance the physical properties of the material. Indeed, a wide range of corresponding experimental studies have been reported.[15–17] For instance, Liu has found that strain in $Co_xZn_{1-x}O$ can enhance ferromagnetism.[15] Gupta has predicted that the op-

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†Corresponding author. E-mail: slb0813@sohu.com

tical properties of semiconductor quantum dots will be strongly affected by the strain due to lattice mismatch between the substrate and deposited material.[16] Our previous studies have also discovered that the strain in thin films can affect electronic transport,[17] leading to increasing surface resistance of the sample. However, the issues about strain affecting the electronic structures and optical properties of $Mg_xZn_{1-x}O$ are not fully understood yet and there is a lack of systemic and theoretical analysis.[15]

In this paper, the electronic structures and optical properties of $Mg_{0.25}Zn_{0.75}O$ will be investigated. The calculation is carried out in a-axis and c-axis strain, changing from 0.3 to –0.2. This paper is organized as follows. Firstly, we describe the details of computation we have carried out. Secondly, we discuss density of states and band structure in axis strain. Finally, we investigate the imaginary part of the dielectric function ε_2 and absorption coefficient α as functions of axis strain.

2. Computational method

In this paper, electronic structures and optical properties of the $Mg_{0.25}Zn_{0.75}O$ are calculated by using CASTEP code which is based on density function theory and plane-wave pseudopotential method.[18] The generalized gradient approximation (GGA) in the scheme of Perdew–Burke–Ernzerhof is applied to describe exchange-correlation potential between electrons.[19] Because previous studies have shown that the norm-conserving pseudopotential is more suitable than the ultrasoft pseudopotential in optical properties,[20] the interaction between valence electron and ion core is described by norm-conserving pseudopotential. The valence electron configurations for Mg, Zn and O are considered as $3s^2$, $3d^{10}4s^2$ and $2s^22p^4$, respectively.

The calculation is performed in the 2×2×1 ZnO supercell, which contains 8 Zn atoms and 8 O atoms. We can obtain $Mg_{0.25}Zn_{0.75}O$ structure by substitution of 2 Mg atoms for 2 Zn atoms in ZnO supercell. The convergence tests of the total energy with respect to the plane wave energy cutoff and k-points sampling have been carefully examined (see Table 1). As seen from Table.1, the total energy hardly changes when the energy cutoff is 600 eV. The final set of energy is computed with an energy cutoff of 600 eV for the $Mg_{0.25}Zn_{0.75}O$ and the integration is performed using $4 \times 4 \times 4$ k-point sampling which is generated by the Monkhorst-Pack scheme. The strain from a-axis and c-axis is defined as[21]

$$\varepsilon = (c - c_0)/c_0 \times 100\%. \quad (1)$$

Here c is lattice constant of strained $Mg_{0.25}Zn_{0.75}O$ and c_0 is the lattice constant of unstrained $Mg_{0.25}Zn_{0.75}O$. Firstly, we optimize the crystal structure of $Mg_{0.25}Zn_{0.75}O$ with the strain from a-axis and c-axis, and then calculate its density of states, band structures and optical properties.

Table 1. Geometry optimization of $Mg_{0.25}Zn_{0.75}O$ at different cut off energy (1Å = 0.1nm).

Cut off energy /eV	a /Å	b /Å	c /Å	Total energy/eV	Volume /Å^3	Band gap/eV
650	3.245	3.245	5.220	−2805.476	47.651	0.95
600	3.245	3.245	5.231	−2805.456	47.780	0.95
550	3.243	3.243	5.235	−2805.371	47.783	0.95
500	3.241	3.242	5.212	−2805.211	47.428	0.92
Ref.[14]	3.250	3.250	5.190	—	47.500	3.85

3. Results and discussion

3.1. The crystal structure

The optimized results of $Mg_{0.25}Zn_{0.75}O$ with strain $\varepsilon = 0$ are presented in Table.1. Values of lattice constant and cell volume obtained with energy cutoff of 600 eV are comparable to the experimental results obtained from Ref.[14]. The lattice constant a is a little smaller than the value reported in the literature and b is a little larger than that reported in the literature. The error is less than 0.8%, indicating that the calculated method applied in this paper is rational. The ratio of c/a is 1.612, which is equivalent to the value of ZnO 1.602 reported in Ref.[13] and a little smaller than the value of ideal hexagon crystal structure in closest packing, 1.633.[22]

The band gap calculated from GGA is 0.95 eV, which is less than experimental value 3.85 eV.[14] It

is well known that the band gap is underestimated due to neglect of correlation between excited state electrons.[23,24] In this paper, the scissor operation is defined as the difference between experimental value 3.85 eV and calculated value 0.95 eV, which is 2.9 eV.

3.2. Electronic properties

Figure 1 shows the density of states of $Mg_{0.25}Zn_{0.75}O$ in a-axis strain. For $\varepsilon = 0$, the density of states in the range from –17.0 eV to –15.5 eV comes from O 2s, which is regarded as lower valence band. The density of states in the range from –6.5 eV to 0 eV mainly comes from Zn 3d and O 2p, which is regarded as upper valence band. The results are consistent with previous calculation.[25] Zn 3d has main contribution to bottom of upper valence band, and O 2p has main contribution to top of upper valence band.

Variations of band gap for $Mg_xZn_{1-x}O$ have been investigated in previous studies when Mg substitutes for Zn.[7] Yadav[9] pointed out that the bonding between Zn atoms will be strengthened and will lead to a larger overlap between tight-binding basis orbitals when Mg substitutes for Zn, which affects the variation of band gap. Jin[13] considered that bonding between Zn and O atoms would be weakened when Mg substituted for Zn, which would lead to broadening of band gap. However, the issue about strain affecting the variation of band gap in $Mg_xZn_{1-x}O$ is lack of systemic analysis now. Here we mainly analyse and discuss the strain effect on density of states and band structure of $Mg_{0.25}Zn_{0.75}O$. It is clearly seen from Fig.1 that the partial density of states for O 2s,

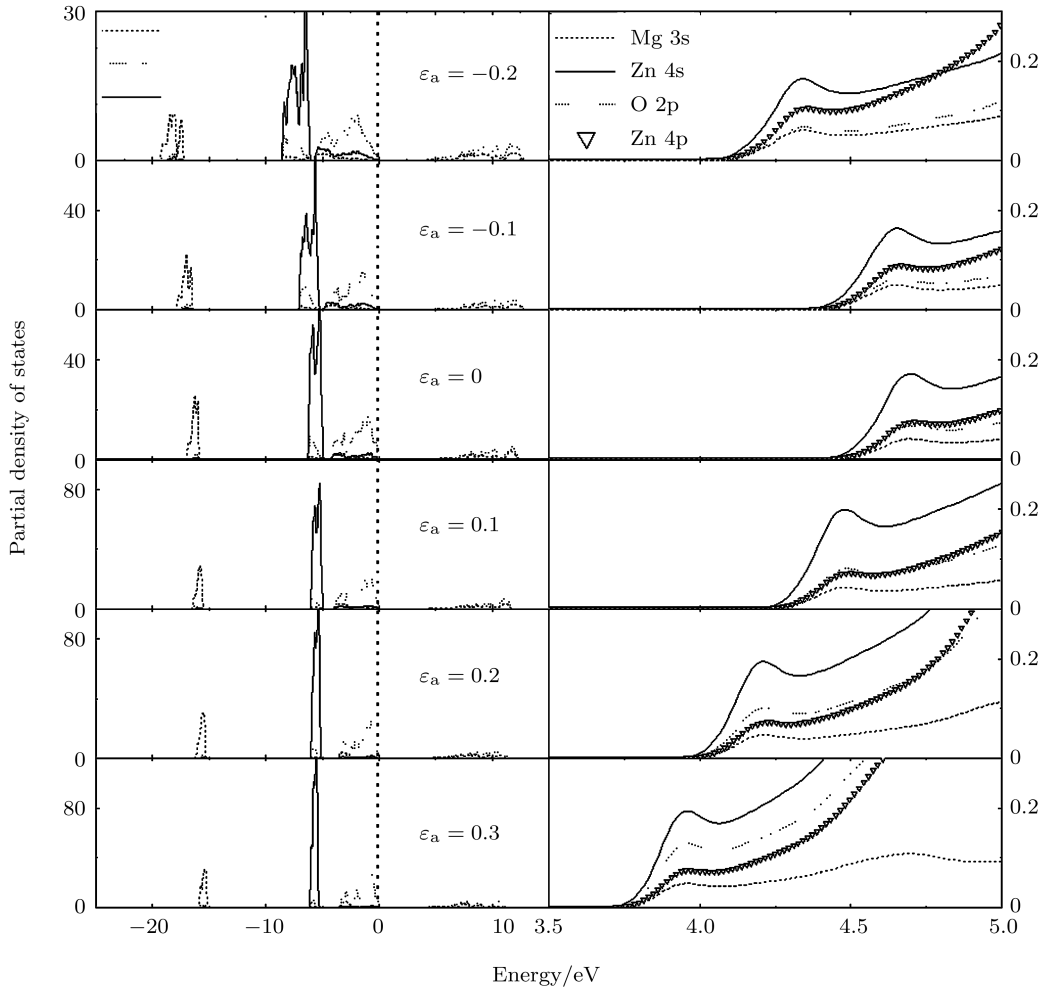


Fig.1. Partial density of states for $Mg_{0.25}Zn_{0.75}O$ in a-axis strain changing from 0.3 to –0.2. The right-hand side of the figure shows the partial density of states near the bottom of conduction band. Dotted line is the top of valence band.

O 2p and Zn 3d shifts to the lower energy range when strain changes from 0.3 to –0.2. Besides, it can also be observed that Zn 3d and O 2s have stronger non-local characteristic and show a splitting when strain changes from 0.3 to –0.2. It is necessary to point out that the valence band near 0 eV has no obvious shift and the top of valence band is always dominated by O 2p when strain changes. The results cannot be fully verified yet by corresponding experiments due to present technique limitation.[15] It is clearly seen from Fig.1 that the conduction band is dominated by Mg 3s, Zn 4s, O2p and Zn 4p. But the bottom of conduction band is always dominated by Zn 4s, which shifts to higher energy range when strain changes from 0.3 to 0, and then shifts to lower energy range when strain changes from 0 to –0.2. The shift leads to variation of band gap and provides a new method for the application of $Mg_xZn_{1-x}O$.[6,7] It is necessary to point out that the band gap is always dominated by Zn 4s and O 2p, which has also been found previously in ZnO.[25]

Figure 2 shows the density of states of $Mg_{0.25}Zn_{0.75}O$ in *c*-axis strain. The variation of valence band for strain in *c*-axis is similar to that in *a*-axis. It is seen form Fig.2 that the bottom of conduction band is always dominated by Zn 4s and shifts to higher energy range when strain changes from 0.3 to –0.2. The difference of density of states between *a*-axis and *c*-axis strain reflects the anisotropy of electron cloud distributed in space for $Mg_{0.25}Zn_{0.75}O$. Figure 3 shows the density of states near the top of valence band. It is clear from Fig.3 that the density of states increases with *a*-axis strain changing from –0.2 to 0.3. But the density of states has no clear variation with the change of *c*-axis strain.

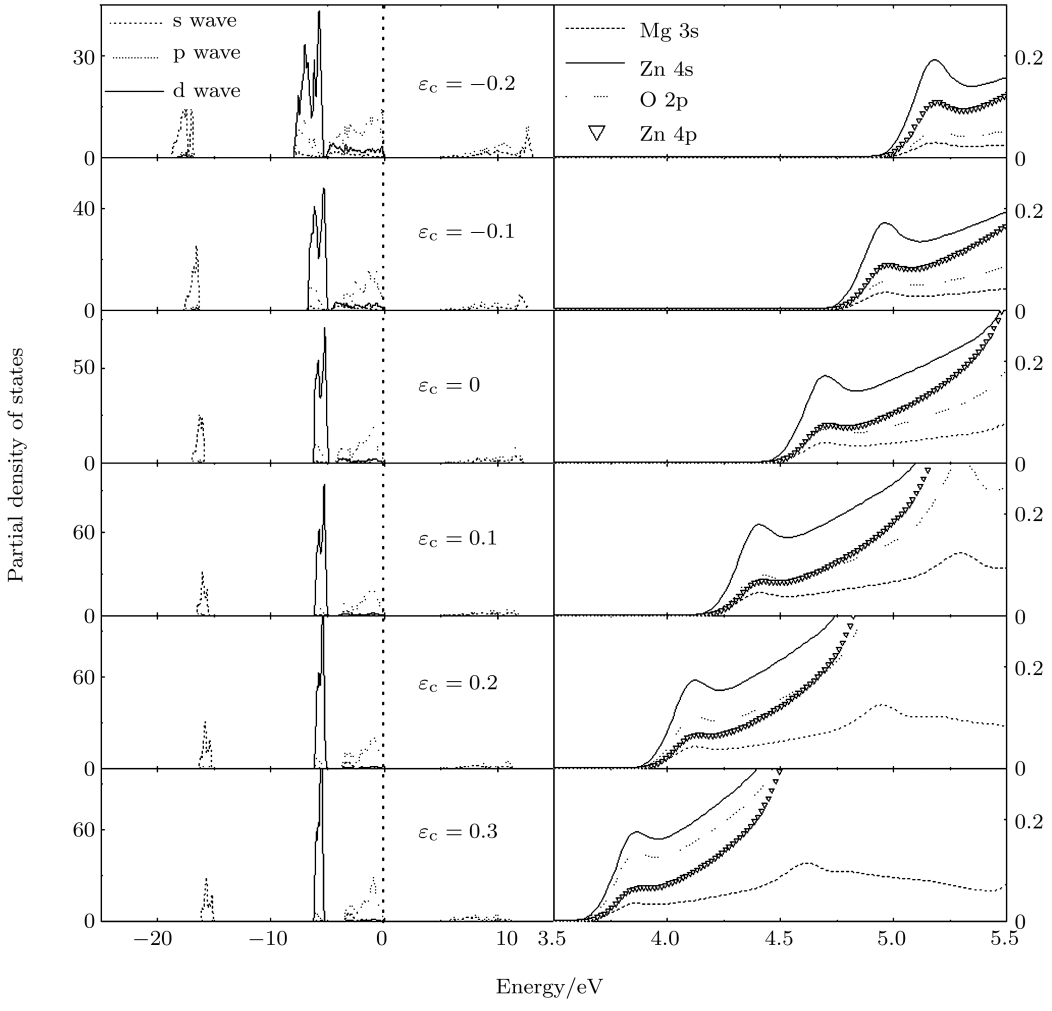


Fig.2. Partial density of states for $Mg_{0.25}Zn_{0.75}O$ in *c*-axis strain changing from 0.3 to –0.2. The right-hand side of the figure shows the partial density of states near the bottom of conduction band. Dotted line is the top of valence band.

In view of valence electrons of Mg-$3s^2$, Zn-$3d^{10}4s^2$ and O-$2s^22p^4$, there are 124 states for the $Mg_2Zn_6O_8$ under valence band if the electrons are in the assigned valence states. The number of states in upper valence band is 108, obtained by integration of the density of states in the upper valence band[26] (see Table 2). We also calculate the number of Zn 3d states and O 2p states in upper valence band. It can be seem from Table.2 that the number of states in upper valence band does not change with strain. But the number of Zn 3d states will slightly reduce and the number of O 2p states will slightly increase when strain changes in the range from 0.3 to –0.2.

Table 2. The states in upper valence band for Zn 3d and O 2p, and the percent of Zn 3d and O 2p in upper valence band for a-axis and c-axis strains (a-axis strain / c-axis strain).

Strain	States	Zn 3d	O 2p	Percent (Zn 3d)	Percent (O 2p)
–0.2	108.000/108.000	59.006/59.002	40.696/40.907	0.546/0.546	0.377/0.379
–0.1	108.000/108.000	59.367/59.386	40.526/40.571	0.550/0.550	0.375/0.376
0	108.000	59.523	40.316	0.551	0.373
0.1	108.000/108.000	59.616/59.603	40.059/40.058	0.552/0.552	0.371/0.371
0.2	108.000/108.000	59.654/59.636	39.833/39.813	0.552/0.552	0.369/0.369
0.3	108.000/108.000	59.671/59.658	39.616/39.543	0.552/0.552	0.367/0.366

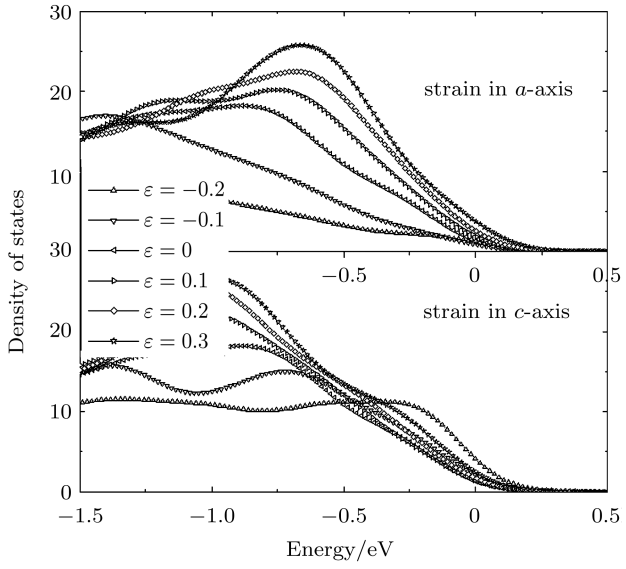


Fig.3. Density of states near the top of valence band for $Mg_{0.25}Zn_{0.75}O$.

The calculated band structures for $Mg_{0.25}Zn_{0.75}O$ are shown in Fig.4. There is a direct gap of 3.85 eV from top of upper valence band (G point) to bottom of conduction band (G point). The scissor operation applied in the calculation is 2.9 eV. This result can be verified by experiment in Ref.[14]. As seen from Fig.4, the top of upper valence band is flat by comparing to the bottom of conduction band near G point, suggesting that the cavity near the top of upper valence band has larger effective mass. This is a possible reason that it is difficult to obtain p-type ZnO by doping.[25] The $Mg_{0.25}Zn_{0.75}O$ is still a direct band gap semiconductor

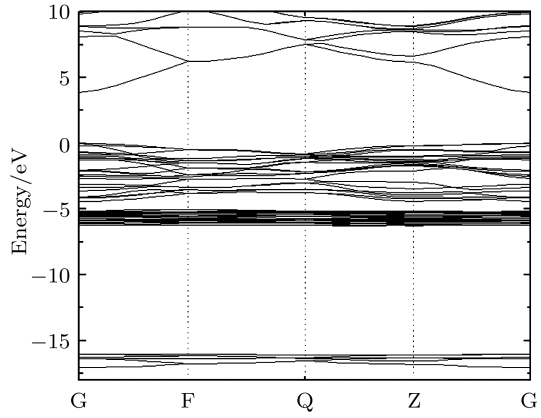


Fig.4. Calculated band structures for $Mg_{0.25}Zn_{0.75}O$ with strain $\varepsilon = 0$ (the scissor operation is 2.9 eV).

when strain changes. The band gap varies with strain. The values of band gap calculated from band structure are shown in Fig.5, in which the band gaps calculated

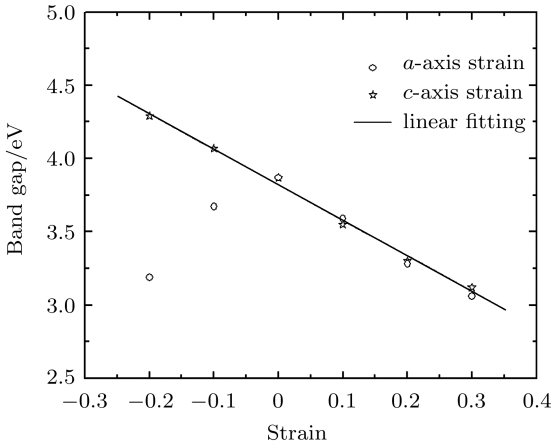


Fig.5. The variation of band gap with strain, calculated from band structure for $Mg_{0.25}Zn_{0.75}O$.

from c-axis strain vary linearly with the strain, and can be fitted by a polynomial $E_g = A\varepsilon + B$ with parameters $A = -2.42\,\text{eV}$ and $B = 3.82\,\text{eV}$. In the previous experiment,[27] Li proved that band gaps obtained from absorption edge of ZnO also vary linearly with biaxial stress. The variation of band gap is abnormal for a-axis strain changing from 0 to –0.2, which may come from Zn 4s shift to lower energy range.

3.3. Optical properties

It is well known that the interaction between electron and photon can be described according to time-dependent perturbation of the electron states. Electron transition between occupied and unoccupied states can be caused by the electronic field of photon. Because the imaginary parts of dielectric function ε_2 and absorption coefficient α are related to electron transition, it is important to investigate them. They can be described as[28]

$$\varepsilon_2(\omega) = \frac{e^2\pi^2h^2}{\varepsilon_0 m^2(h\omega - \Delta s)^2}\sum_{\text{V.C}}\left\{\int_{\text{BZ}}\frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^3}\left|\boldsymbol{\alpha}\cdot\boldsymbol{M}_{\text{v.c}}\right|^2\delta[E_{\text{C}}(\boldsymbol{k}) + \Delta s - E_{\text{V}}(\boldsymbol{k}) - h\omega]\right\}, \tag{2}$$

$$\alpha = \frac{\omega}{\varepsilon_0}\frac{e^2\pi^2h^2}{ncm^2(h\omega - \Delta s)^2}\sum_{\text{V.C}}\left\{\int_{\text{BZ}}\frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^3}\left|\boldsymbol{\alpha}\cdot\boldsymbol{M}_{\text{v.c}}\right|^2\delta[E_{\text{C}}(\boldsymbol{k}) + \Delta s - E_{\text{V}}(\boldsymbol{k}) - h\omega]\right\}. \tag{3}$$

Here $\boldsymbol{\alpha}$ stands for unit vector, $\boldsymbol{M}_{\text{v.c}}$ stands for transition matrix element, C stands for conduction band, V stands for valence band, BZ stands for Brillouin zone, Δs stands for scissor operation ($\Delta s = 2.9\,\text{eV}$ in this paper), e is charge of electron, ε_0 is vacuum dielectric constant, m is electron mass, ω is photon frequency, h is Planck constant, $\boldsymbol{k}$ is wave vector, n is refractive index and c is velocity of light. It is seen from Fig.6 that there are three main peaks for $Mg_{0.25}Zn_{0.75}O$ in a-axis or c-axis strain. When strain $\varepsilon = 0$, the peaks are 4.5 eV (1.6+2.9 eV), 9.6 eV (6.7+2.9 eV), 13.3 eV (10.4+2.9 eV), respectively. The peak at 4.5 eV should be mainly caused by electronic transition between O 2p in upper valence band and Zn 4s in conduction band, and it is not far from the direct band gap of 3.85 eV (0.95+2.9 eV) obtained from band structure. The peak at 9.6 eV should be caused by electronic transition between Zn 3d and O 2p and the third peak at 13.3 eV should be caused by optical transition between Zn 3d and O 2s. The electronic transitions are consistent with previous results reported in Ref.[29]. We can see clearly that the first peak shifts from 4.32 to 4.47 eV when a-axis strain changes from 0.3 to 0, and then shifts from 4.47 to 4.10 eV when a-axis strain changes from 0 to –0.2. But the first peak shifts from 3.68 to 5.14 eV when c-axis strain changes from 0.3 to –0.2. The results are qualitative in agreement with the previous conclusion from density of states. Other peaks are also seen in Fig.6, which cannot be analysed quantitatively now and need be verified by further experiments.

Figure 7 shows the optical absorption edge of $Mg_{0.25}Zn_{0.75}O$ with strain. We can see from Fig.7 that the absorption edge is blue-shifted when c-axis strain changes from 0.3 to –0.2. But the absorption edge is red-shifted when a-axis strain changes from 0 to –0.2. It is well known that the relation between the optical band gap and the absorption coefficient α is given by[30]

$$\alpha h\upsilon \propto (h\upsilon - E_g)^{0.5}. \tag{4}$$

Here υ is the frequency of radiation. The optical band gap can be obtained from the intercept of $\alpha h\upsilon$ versus photon energy $h\upsilon$. Figure 8 shows optical band gap of $Mg_{0.25}Zn_{0.75}O$. This band gap obtained from absorption coefficient is approximatively equal to the result from the band structure. For $\varepsilon = 0$, the optical band gap is $E_g = 3.77\,\text{eV}$, and the corresponding wave length of photons is $\lambda = 332\,\text{nm}$. The result is consistent with the experimental value ($\lambda = 333\,\text{nm}$ for $Mg_{0.24}Zn_{0.76}O$) reported in Ref.[31]. We fit the optical band gap obtained from c-axis straining, using a polynomial $E_g = A\varepsilon + B$ with parameters $A = -2.69\,\text{eV}$ and $B = 3.80\,\text{eV}$. It is very important to tune optical band gap for application of the $Mg_xZn_{1-x}O$, which has been reported in Refs.[6–8]. But we still need do a lot of experimental researches in order to realize the optical band gap tuned by strain or stress.

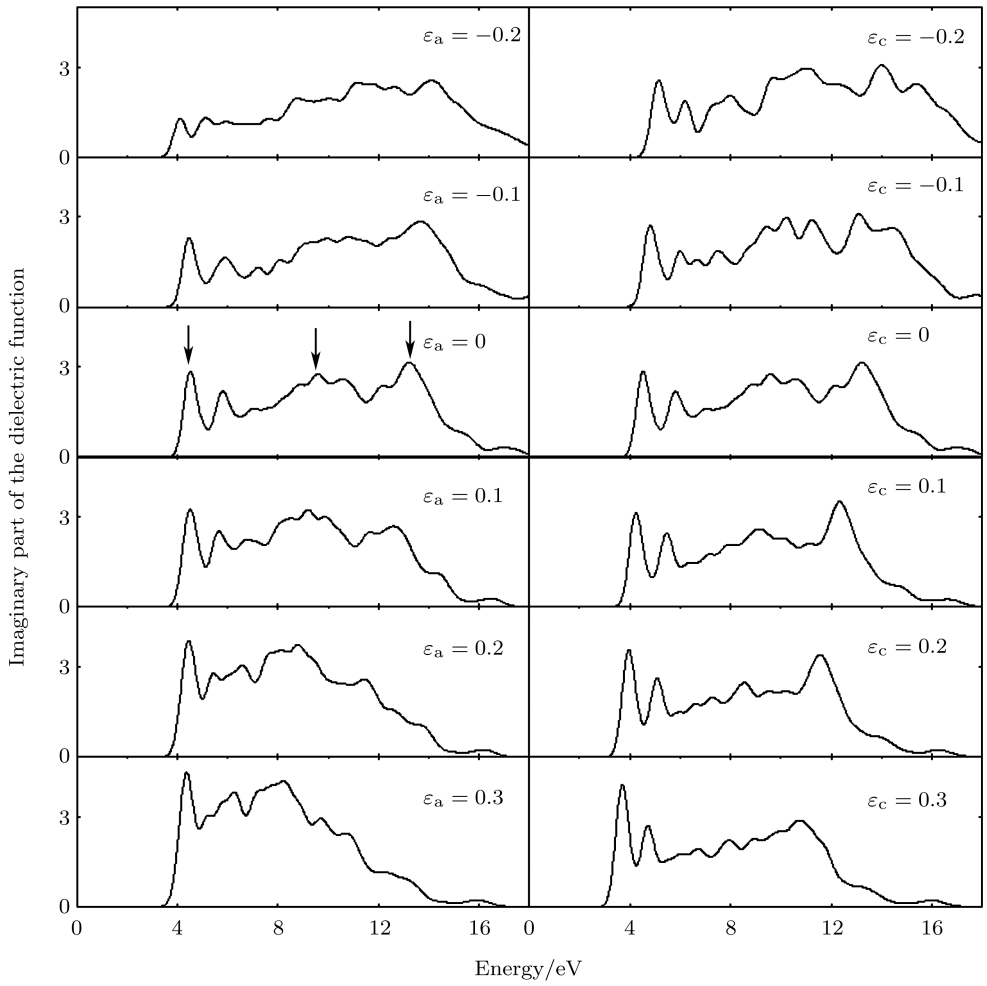


Fig.6. The imaginary part of the dielectric function for $Mg_{0.25}Zn_{0.75}O$ in strain.

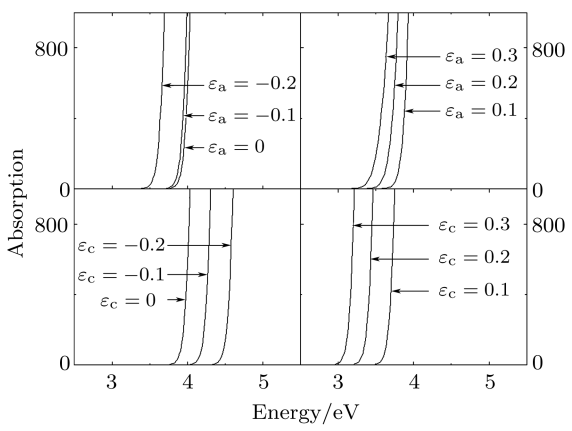


Fig.7. Optical absorption edge for $Mg_{0.25}Zn_{0.75}O$ with strain.

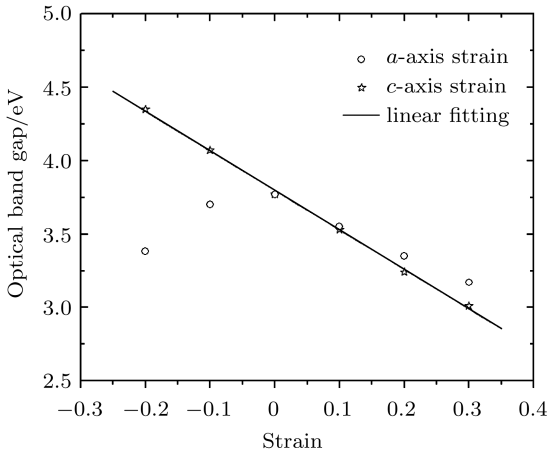


Fig.8. The variation of optical band gap with strain for $Mg_{0.25}Zn_{0.75}O$.

4. Conclusion

When the a-axis and c-axis strain changes in the range from –0.2 to 0.3 in intervals of 0.1, the calculated results from density of states show that the top of valence band is dominated by O 2p and the bottom of conduction band is dominated by Zn 4s. Zn 4s will shift to higher energy range when a-axis strain changes in the range from 0.3 to 0, and then shift to lower energy range when a-axis strain changes in the range from 0 to –0.2. Zn 4s will always shift to higher energy range when c-axis strain changes in the range from 0.3 to –0.2. Variation of the band gap for $Mg_{0.25}Zn_{0.75}O$ can be obtained by band structure and absorption spectra, the result of which is consistent with that calculated from density of states.

References

[1] Liu C H, Liu B C and Fu Z X 2008 *Chin. Phys.* **17** 2292

[2] Polyakov A Y, Smirnov N B, Govorkov A V, Kozhukhova E A, Belogorokhov A I, Kim H S, Norton D P and Pearton S J 2008 *J. Appl. Phys.* **103** 083704

[3] Xiao Z Y, Liu Y C, Mu R, Zhao D X and Zhang J Y 2008 *Appl. Phys. Lett.* **92** 052106

[4] Yun E J, Park H S, Lee, K H, Nam H G and Jung M 2008 *J. Appl. Phys.* **103** 073507

[5] Gai Y Q, Yao B, Wei Z P, Li Y F, Lu Y M, Shen D Z, Zhang J Y, Zhao D X, Fan X W, Li J and Xia J B 2008 *Appl. Phys. Lett.* **92** 062110

[6] Xiao Z, Matsui H, Hasuike N, Harima H and Tabata H 2008 *J. Appl. Phys.* **103** 043504

[7] Li Y F, Yao B, Lu Y M, Li B H, Gai Y Q, Cong C X, Zhang Z Z, Zhao D X , Zhang J Y, Shen D Z and Fan X W 2008 *Appl. Phys. Lett.* **92** 192116

[8] Zhang X D, Guo M L, Li W X and Liu C L 2008 *J. Appl. Phys.* **103** 063721

[9] Yadav M K, Ghosh M, Biswas R, Raychaudhuri A K and Mookerjee A 2007 *Phys. Rev.* B **76** 195450

[10] Sadofev S, Schäfer P, Fan Y H, Blumstengel S and Henneberger F 2007 *Appl. Phys. Lett.* **91** 201923

[11] Tang X, Lu H F, Ma C Y, Zhao J J and Zhang Q Y 2008 *Acta Phys. Sin.* **57** 1066 (in Chinese)

[12] Huang D, Shao Y Z, Chen D H, Guo J and Li G X 2008 *Acta Phys. Sin.* **57** 1078 (in Chinese)

[13] Jin X L, Luo S Y, Kong D G, Li Y C and Du Z L 2006 *Acta Phys. Sin.* **55** 4809 (in Chinese)

[14] Ohomo A, Kawasaki M, Koida T, Masubuchi K, Koinuma H, Sakurai Y and Segawa Y 1998 *Appl. Phys. Lett.* **72** 2466

[15] Liu X J, Song C, Zeng F, Pan F, He B and Yan W S 2008 *J. Appl. Phys.* **103** 093911

[16] Gupta S K, Kapoor S, Kumar J and Sen P K 2007 *Nanotechnology* **18** 325402

[17] Shi L B, Zheng Y, Ren J Y, Li M B and Zhang G H 2008 *Acta Phys. Sin.* **57** 1183 (in Chinese)

[18] Perdew J P, Burke K and Ernzerhof M 1996 *Phys. Rev. Lett.* **77** 3865

[19] Payne M C, Teter M P, Allan D C, Arias T A and Joannopoulos J D 1992 *Rev. Mod. Phys.* **64** 1045

[20] Sun J, Zhou X F, Fan Y X, Chen J, Wang H T, Guo X, He J and Tian Y 2006 *Phys. Rev.* B **73** 045108

[21] Hur T B, Hwang Y H, Kim H K and Lee I J 2006 *J. Appl. Phys.* **99** 064308

[22] Zhang F, Deng Z, Yan J and Zhang Z 2006 *Acta Opt. Sin.* **26** 1203 (in Chinese)

[23] Anisimov V I, Aryasetiawan F and Lichtenstein A I 1997 *J. Phys.*: *Condens. Matter.* **9** 767

[24] Vispute R D, Talyansky V and Choopun S 1998 *Appl. Phys. Lett.* **73** 348

[25] Duan M Y, Xu M, Zhou H P and Shen Y B 2007 *Acta Phys. Sin.* **56** 5359 (in Chinese)

[26] Johnsen S, Bentien A, Madsen G K H, Iversen B B and Nygren M 2006 *Chem. Mater* **18** 4633

[27] Li Y F, Yao B, Lu Y M, Cong C X, Zhang Z Z, Gai Y Q, Zheng C J, Li B H, Wei Z P, Shen D Z and Fan X W 2007 *Appl. Phys. Lett.* **91** 021915

[28] Ying X J, Zhang X D and Hao Z W 2007 *J. Synthetic Crystals* **36** 784 (in Chinese)

[29] Shen Y B, Ming X, Ding Y C, Duan M Y, Linghu R F and Zhu W J 2007 *Acta Phys. Sin.* **56** 3440 (in Chinese)

[30] Serpone N, Lawless D and Khairutdinov R 1995 *J. Phys. Chem.* **99** 16646

[31] Sharma A K, Narayan J, Muth J F, Teng C W, Jin C, Kvit A, Kolbas R M and Holland O W 1999 *Appl. Phys. Lett.* **75** 3327