Article ID: 1000-7032(2022)02-0218-08

Local Electronic Structure of Lithium Nitrogen Codoped ZnO Films Revealed by X-ray Absorption Fine Structure Spectroscopy

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Abstract: It is to reveal the formation mechanism of Li and N codoped p-ZnO films and the cause for the stable p-type conductivity. The films has been studied by investigating their local electronic structures using X-ray photoelectron spectroscopy and X-ray absorption fine structure spectroscopy based on synchrotron radiation source. The signals of Li—N bond and Li—N complex acceptors in the p-ZnO films have been collected, and the acceptor level estimated from photoluminescence spectroscopy is about 122 meV. The formation of Li—N complex acceptors has been confirmed, and the realization of Li—N bond has been attributed to the origin of the good stability of the p-type ZnO films obtained by Li, N codoping method.

Key words: zinc oxide; p-type doping; formation mechanism; stability; X-ray absorption fine structure spectroscopy
CLC number: O484.4 **Document code**: A **DOI**: 10.37188/CJL.20210365

X 射线吸收谱测算锂氮共掺杂氧化锌薄膜局域电子结构

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摘要: 为了实现对 Li—N 共掺杂 p 型 ZnO 薄膜的形成机制以及其稳定 p 型导电原因的揭示,利用 X 射线光电子谱及基于同步辐射光源的 X 射线吸收精细结构谱测试对薄膜的局域电子结构进行了测算分析。获得了 Li—N 成键及 Li—N 复合型受主形成的信号,利用光致发光测量计算其受主能级为 122 mV。证实了薄膜中 Li—N 复合型受主的形成,而 Li—N 共掺杂 p 型 ZnO 良好的稳定性则归因于 Li—N 共掺杂在 p 型 ZnO 薄膜中实现了 Li 和 N 的成键。

关 键 词: 氧化锌; p 型掺杂; 形成机制; 稳定性; X 射线吸收精细结构谱

收稿日期: 2021-11-17; **修订日期**: 2021-12-07
基金项目: 国家自然科学基金(61704065,61705078,11904130)资助项目
Supported by National Natural Science Foundation of China(61704065,61705078,11904130)

1 Introduction

Zinc oxide(ZnO) has attracted much attention for its potential applications in ultraviolet light-emitting devices and low-threshold lasers, *etc*[1-4]. In order to realize the optoelectronic application of ZnO, the realization of both n- and p-type conductivity in ZnO is demanded. Undoped ZnO is usually n-type, whereas the stable and reproducible p-type ZnO is rather difficult to obtain due to the relatively high ionization energy of acceptor impurities, low solubility of dopants, and self-compensation effect in ZnO[5-6]. To date, numerous efforts have been paid to this issue, and p-type ZnO films have been demonstrated using many different acceptor dopants[7-12]. However, the reproducibility and stability of the p-type ZnO films are still poor, which cast a heavy shadow on whether real p-type films have been realized, and whether the p-type films are applicable to optoelectronic devices[13-14]. Based on the local density approximation calculations, Li and N impurities are the best candidates for creating p-type ZnO in regard to the strain effect and energy levels[15]. However, there are still some problems to be solved. The incorporated N may occupy O sites to form the nitrogen substituted oxygen (N_O) acceptors, but the solubility of N in ZnO is too low to generate enough N_O acceptors, moreover the N ions in ZnO may integrate together to form N_2-on-O substitutions $(N_2)_O$ donors[16-17]. Li can be easily induced into ZnO, and Li substituted Zn (Li_{Zn}) can act as acceptors, but the Li may also occupy the interstitial sites (Li_i) acting as the Li_i donors or the Li_{Zn}—Li_i complex donors[18-19]. For the above reasons, the reproducibility and stability of p-type ZnO doped by single N or Li are poor. In the past few years, a Li and N codoping method has been employed for the p-type doping of ZnO[20-23]. On one hand, the Li—N codoping may form multiform acceptors such as Li_{Zn}, N_O and some complex acceptors. On the other hand, it is expected to bond Li with N that may depress the migration of N and Li to decrease the production of $(N_2)_O$ and Li_i related donors and suppress the compensation for the existing acceptors. Some reports have demonstrated the reproducible and stable p-type ZnO films obtained by the Li, N codoping method, and devices that can operate continuously for hours, ultraviolet photodetectors that can still work after several months have been demonstrated, indicating the good stability of the p-type ZnO films[24-27]. However, the formation mechanism and the cause for the stable p-type conductivity have not been revealed yet.

In this paper, the acceptor state of the p-type ZnO films obtained by Li, N codoping method has been studied by investigating the local electronic structures of the films using X-ray absorption fine structure(XAFS) spectroscopy based on synchrotron radiation source, and such a technique has been widely employed to study the local electronic structures of ZnO[28-31]. The formation of Li—N complex acceptors has been confirmed by extended X-ray absorption fine structure(EXAFS) measurements, and the Li—N complex has been attributed to the cause of the stable p-type ZnO films obtained by Li, N codoping method.

2 Experiments

The films investigated in this paper were all grown with a VG V80H radio-frequency molecular beam epitaxy technique employing *a*-plane sapphire as the substrates, and the detailed growth conditions can be found elsewhere[24,26]. Briefly, the p-type ZnO: (Li, N) films were grown with the O source and N dopant from the cracked nitric oxide gas in an Oxford Applied Research plasma cell(Model HD25) at a fixed radio-frequency power of 330 W, and Zn source and Li dopant are leading into the growth chamber from heating metallic zinc and lithium in individual Knudsen cells at 240 ℃ and 310 ℃, respectively. For comparison, single N, single Li and undoped ZnO films were prepared under the same growth conditions. The chemical bonding states in the ZnO films were analyzed in an AXIS Ultra "DLD" X-ray photoelectron spectrometer (XPS). EXAFS spectra of Zn K-edge were collected at the X-ray Absorption Fine Structure station (Beam line 14 W1) of Shanghai Synchrotron Radiation Facility

(SSRF) using the fluorescence mode at room temperature. Temperature dependent photoluminescence (PL) measurement was performed in a JY-630 micro-Raman spectrometer employing the 325 nm line of a He-Cd laser as the excitation source.

3 Results and Discussion

Fig. 1 shows the XPS data of the ZnO:(Li,N) film. In Fig. 1(a), a Li 1s peak was evidenced at 55.4 eV, which is close to the binding energy of Li in Li—N bonds(55.0 eV) and Li—O bonds(55.6 eV)[32-33]. No signal from Li_i (52.9 eV) can be found[34], revealing that the incorporated Li may occupy Zn sites to form the acceptors Li_{Zn} bonding with N and/or O, while the Li_i that is frequently observed in Li doped ZnO has been depressed in our case. The N 1s spectrum shown in Fig. 1(b) can be fitted using two Gaussian lineshapes at 396.7 eV and 398.7 eV, and the former has been usually attributed to N_O, while the latter is close to the binding energy of Li—N bonds in Li—N complex[20,32]. One can deduce from the above data that Li—N bonds form in the ZnO:(Li,N) films. Thus, it is rational to speculate from the XPS data that the acceptor formed in ZnO:(Li,N) film may be the Li—N complex containing Li_{Zn} and N_O.

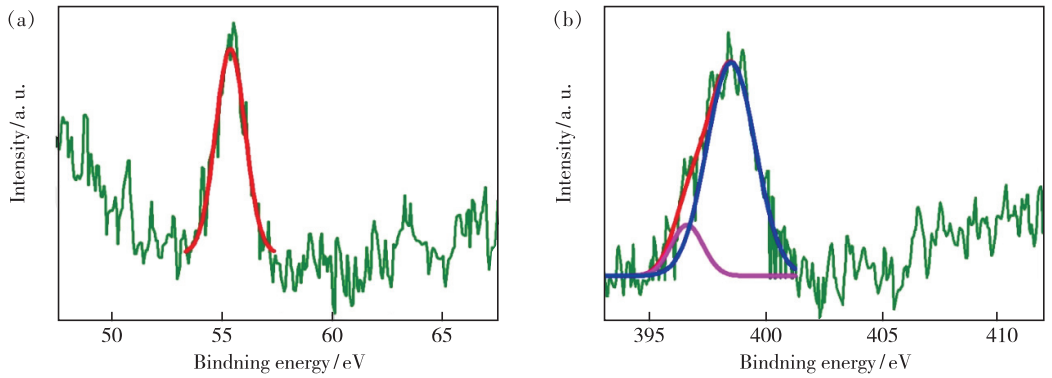

Fig. 1 XPS spectra of Li 1s(a) and N 1s(b) in ZnO:(Li,N) films. Note that the spectra have been fitted using Gaussian line shapes.

In order to further prove the above speculation, the Zn K-edge EXAFS absorption spectra of ZnO:(Li,N), ZnO:N, ZnO:Li and ZnO films were measured, as shown in Fig. 2(a). The inset shows the amplified profile of the near-edge feature, attributed to the unoccupied hybridized O 2p and Zn 4sp orbits, with a large ratio of p_{xy} states to p_z states. Interestingly, doping of Li, N or Li—N increases the near-edge peak intensity, which could indicate the localization of the conduction band through limited hopping interactions and orbital hybridization between adjacent ions, upon the inducing of the dopants. The Zn K-edge EXAFS spectra were analyzed by the programs of Athena V0.8.056, Artemis V0.8.012 within the IFEFFIT package[34-36] version 1.2.11. Fig. 2(b) shows the $\boldsymbol{k}^3$-weighted $\chi(\boldsymbol{k})$ signal of EXAFS data(a function of the photoelectron wave-vector $\boldsymbol{k}$), which reflects the scattering effects from other atoms around the given atom. The intensity of $\chi(\boldsymbol{k})$ can be related to the coordination number of Zn atoms. The EXAFS data were Fourier-transformed to R space and fitted to the theoretical EXAFS calculations, as shown in Fig. 2(c). The first shell of the radial distribution function indicates the position of the Zn—O bond distance, and the second shell peak denotes a combination of Zn—Zn bond distances. It is interesting to observe that, the Zn—O bond length in ZnO:(Li,N) is slightly shorter than that in ZnO:N, ZnO:Li and ZnO, which reveals that the substituted site doping by the Li plus N elements will produce the change of the localized structure. One can speculate that Zn—O bond length will be increased if $(N_2)_O$ or Li_i is dominant because either of them will then be pushed O atom and the Zn atoms away from their original sites, increase the Zn—O bond length. Only the bond of Li_{Zn} and N_O as shown in XPS results may decrease the Zn—O bond length, for the length of Li—N bond is

shorter than that of Zn—O bond. While its Zn—Zn bond length is almost invariable for all cases, as labeled by the red line. This result indicates that doping whether it is acceptor or donor does not change the total volume. The predicted bond length is under estimated from their actual bond lengths due to the phase shift of the backscattered photoelectrons. In our case, relative change is of greater importance than actual values. Detailed bonding analysis (summarized in Tab. 1) was conducted with a $\boldsymbol{k}$ range of 20 – 125 nm^{-1} and R range of 0.1 – 0.36 nm. The fitting included single- and multi-scattering paths, with 95% polarization of the incident X-rays taken into account. A fully occupied wurtzite model (space group: $P63m$) with $a = 0.324\ 9$ nm and $b = 0.520\ 7$ nm was used while taking into account four different scattering paths[37] (namely Zn—O1, Zn—O2, Zn—Zn1 and Zn—Zn2), according to symmetry of the structure (the paths of Zn—O1 and Zn—O2 are illustrated in Fig. 2(d)). During the fitting, varied parameters include bond length R, coordination number N, and the Debye-Waller factor σ^2, which includes thermal vibrations and static disorders and is set the same for Zn—O1 and Zn—O2, and the same for Zn—Zn1 and Zn—Zn2. As shown in Fig. 2(d) and Tab. 1, for ZnO: (Li,N), there is about 0.015 nm of bond length difference between Zn—O1 and Zn—O2, while for the bond length difference is only 0.002 nm for ZnO: N, ZnO: Li and ZnO. This indicates that, the symmetry of the original ZnO structure has been deviated for the formation of Li—N bond, while the similar effect is not observed in sole N or Li doping condition. The above results are consistent with the speculation shown in the XPS data that N has been bonded with Li and the Li—N complex acceptors have formed in the ZnO: (Li,N) films.

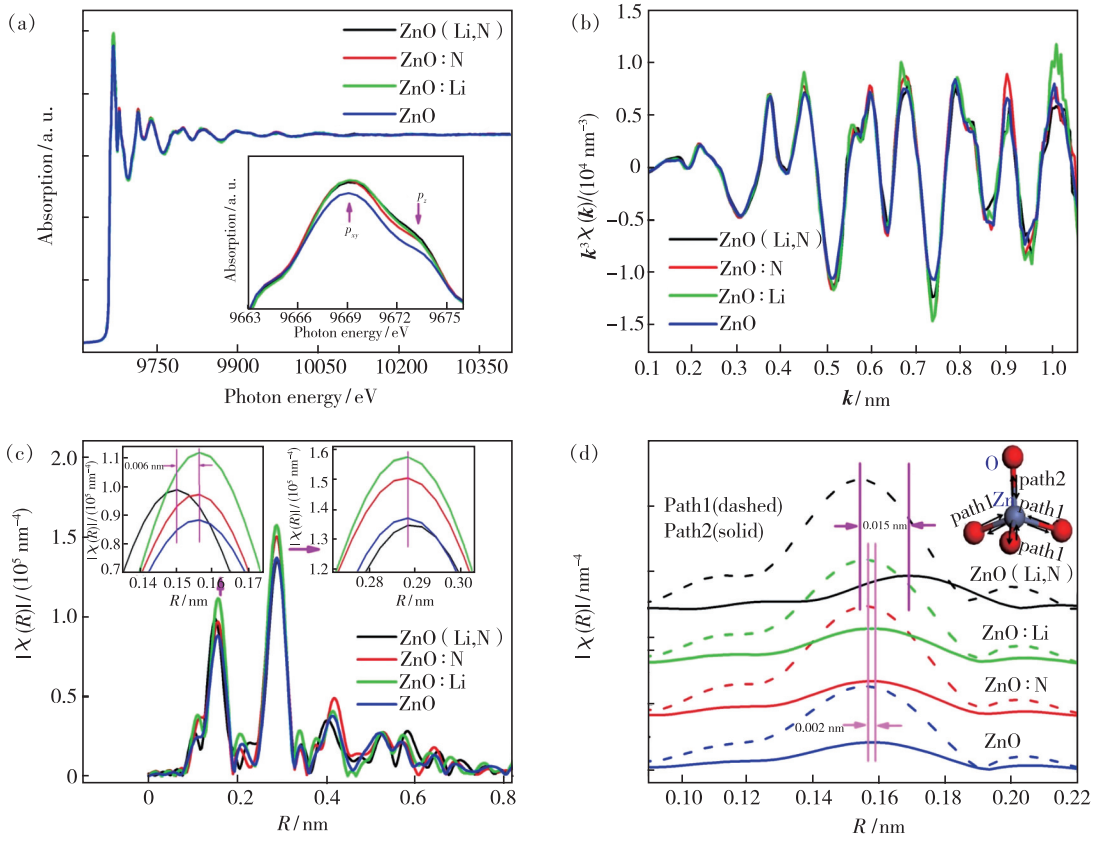

Fig. 2　Zn K-edge X-ray absorption spectra of ZnO: (Li,N), ZnO: N, ZnO: Li and ZnO films. (a) The measured full X-ray absorption spectra. The inset shows the amplified near edge feature with indication of Zn electronic orbital components, namely, p_{xy} and p_z. (b) $k^3\chi(k)$ is represented as a function of $\boldsymbol{k}$. (c) Fourier-transformed EXAFS data in R space, fitted to the theoretical EXAFS calculations. (d) Fitted EXAFS data in R space along Zn—O1 and Zn—O2 paths. The insets show the corresponding atomic geometric structures of the bonds of Zn—O1, Zn—O2.

Tab. 1 Coordination number (N), bond length R, and Debye-Waller factor (σ^2) of ZnO:(Li,N), ZnO:N, ZnO:Li and ZnO films, determined through fitting the orientation-dependent EXAFS data measured at the Zn—K edge

	R-factor	N(Zn—O1)	N(Zn—O2)	σ(Zn—O1)	σ(Zn—O2)	R(Zn—O1)	R(Zn—O2)
Model		3	1			1.973	1.992
ZnO	0.001 01	2.43(0.17)	0.81(0.06)	0.004 6(0.001 5)	0.004 5(0.002 5)	1.972(0.006)	1.991(0.006)
ZnO:N	0.001 2	2.46(0.16)	0.82(0.05)	0.003 3(0.001 0)	0.003 3(0.001 0)	1.966(0.009)	1.984(0.009)
ZnO:Li	0.001 61	2.58(0.42)	0.86(0.14)	0.002 7(0.001 3)	0.002 7(0.001 2)	1.965(0.01)	1.983(0.01)
ZnO:(Li,N)	0.002 60	2.67(0.24)	0.89(0.08)	0.002 5(0.001 3)	0.002 5(0.001 3)	1.943(0.008)	2.089(0.034)

	N(Zn—Zn1)	N(Zn—Zn2)	σ(Zn—Zn1)	σ(Zn—Zn2)	R(Zn—Zn1)	R(Zn—Zn2)
Model	6	6			3.209	3.249
ZnO	5.4(0.24)	5.4(0.24)	0.010 6(0.002 8)	0.007 8(0.001 5)	3.190(0.007)	3.231(0.007)
ZnO:N	5.94(0.66)	5.94(0.66)	0.009 1(0.000 9)	0.009 1(0.000 9)	3.197(0.003)	3.238(0.003)
ZnO:Li	5.94(0.88)	5.94(0.88)	0.011 1(0.004 7)	0.007(0.001 7)	3.189(0.009)	3.229(0.009)
ZnO:(Li,N)	5.34(0.48)	5.34(0.48)	0.008 9(0.005 5)	0.006(0.002 5)	3.153(0.026)	3.251(0.026)

The temperature-dependent PL measurements of ZnO:(Li,N) film are shown in Fig. 3. The spectrum at 80 K consists of three main emission bands, located at 3.315, 3.347, 3.203 eV, respectively. According to their positions, the peak at 3.315 eV can be attributed to electronic radiative transition from conduction band to neutral acceptor level (eFA), the one at 3.347 eV to the emission from neutral acceptor-bound excitons (A^0X), and the broad bands centered at 3.202 eV from the recombination of donor-acceptor pairs (DAP)[22,36]. With the increase of the measuring temperature, the eFA peak at 3.315 eV redshifts, while the DAP peak blueshifts firstly and finally merges into 3.315 eV band at about 140 K. These are the feature of the thermal ionization of donors, which are typical characteristics of transition between DAP and eFA. Since

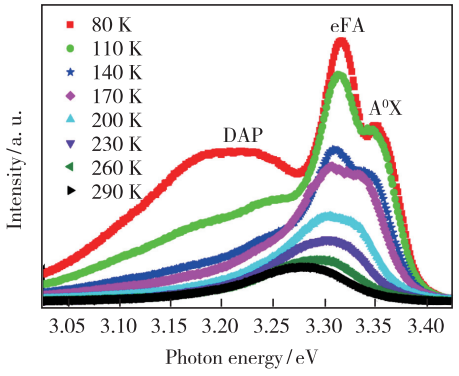

Fig. 3 Temperature-dependent PL spectra of the ZnO:(Li, N) films from 80 K to 290 K

the position of eFA has been ascertained, the acceptor level of the p-type films can be calculated using the following equation[22,36]:

$$E_{FA}(T) = E_g(T) - E_A + kT/2, \quad (1)$$

where $E_g(T)$ is the temperature-dependent band gap following a Varshni-type equation, E_A is acceptor level, k and T are Boltzmann constant and temperature, respectively. Using the eFA emission peak positons and the E_g value at 80 K, the acceptor level can be calculated to be about 122 meV according to Eq. 1. This value is similar to the acceptor level of Li—N complex acceptors reported before (126 meV)[22,36] and different from the single Li_{Zn} (90 or 150 meV)[15,37] or N_O acceptor level (170 – 200 meV)[6]. This result also verifies the speculations from XPS and XAFS measurements that the p-type conductivity of the ZnO:(Li,N) films comes from the contribution of the Li—N complex acceptors containing Li_{Zn} and N_O. The bonding of Li and N may also explain the disappearance of $(N_2)_O$ and Li_i signals in XPS measurements, *i. e.* Li bonding with N depresses the migration of N and Li, suppresses the formation of $(N_2)_O$ and Li_i. Also, it is speculated that the Li—N bonds will suppress the migration of N or Li in the ZnO matrix, thus improve the stability of the p-type ZnO films. It has been demonstrated both theoretically and experimentally that the doping using complex acceptors may be a promising route to p-type

ZnO[38-42]. The results reported in this paper consolidate the above viewpoint.

4 Conclusion

In conclusion, the formation mechanism of Li, N codoped ZnO films has been investigated using X-ray photoelectron spectroscopy and X-ray absorption fine structure spectroscopy based on synchrotron radiation source in this study, and the p-type conductivity is mainly originated from the Li—N complex acceptors as revealed by XPS and XAFS, and the acceptor level was estimated to be about 122 meV. The bonding of Li and N will also suppress the formation of $(N_2)_O$ and Li_i donors and improve the stability of the p-type films. The understanding of acceptor formation and stability mechanisms will be of importance for further improvement of the Li—N codoped p-type ZnO, thus push the development of ZnO optoelectronics forwards.

Response Letter is available for this paper at: http://cjl.lightpublishing.cn/thesisDetails#10.37188/CJL.20210365.

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