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Crystal-Field Symmetry of Luminescence Center in Er-Implanted Silicon

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Abstract A crystal field model for the electronic structure of Er luminescence center in silicon is proposed. Nine photoluminescence spectra of Si : Er and Si : Er, O samples are attributed to the crystal-field splitting of $^4I_{13/2} \rightarrow {}^4I_{15/2}$ transition of Er^{3+} on the sites of tetrahedral symmetry. The oxygen codopants greatly enhance the luminescent output, but similar spectral features appear in both Si : Er and Si : Er, O. From this analysis, we conclude that oxygen codopants do not change the Td symmetry on the site of Er^{3+} doped in silicon.

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1 Introduction

Rare-earth doping of semiconductors has been intensively investigated with a view to its application in optoelectronic devices. The presence of an incompletely filled 4f shell offers the attractive possibility of induced intrashell excitations, largely independent of the surrounding environment. Sharp atomic-like spectra can consequently be generated with the wavelengths being controlled by the dopant itself rather than by the host crystal or temperature. Recently, considerable interest and research effort have been directed towards erbium-doped silicon. This is for two main reasons: firstly, the characteristic of transitions of the erbium ion in the 1.54μm range coincides with the optical window of SiO_2 fibers currently used for telecommunications, and secondly, such a system can be easily integrated with devices manufactured by using the highly successful standard silicon technology[1~5]. Unfortunately, the intensity of the luminescence is very weak. It was found however, that codoping the sample with one of a variety of elements such as oxygen

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greatly enhances the luminescent output. The question has remained as to possible mechanism of the influence of co-doped oxygen. For example oxygen has a strong affinity for electrons, and this may leads to capture of free exciton more efficiently to excite Er ions. Another possibility is that the presence of oxygen around Er^{3+} may reduce the symmetry of the crystal field at the Er site, thereby changing the character of Er wave functions, which may increase the transition probabilities for the luminescence.

2 Symmetry

The Er^{3+} ion has a $4f^{11}$ configuration. The crystal-field splitting model of Er^{3+} on the site of Td symmetry is shown in Fig. 1. According to Hund's rules, the electron-electron interaction results in the ^4I as the ground term; the spin-orbit interaction splits the ^4I term into four manifolds comprising $^4I_{9/2}$, $^4I_{11/2}$, $^4I_{13/2}$ and $^4I_{15/2}$. While $I_{13/2}$ and $^4I_{15/2}$ correspond to the initial excited state and the ground state of Er^{3+} in the free space respectively.

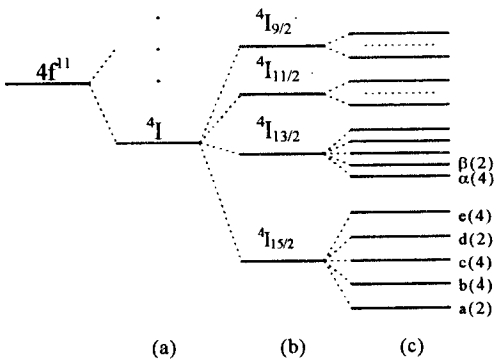

Fig. 1 Crystal-field model for the f^{11} configuration

(a) electron-electron interaction yielding ^4I as the ground state; (b) spin-orbit interaction; (c) the stark levels resulting from crystal-field of Td symmetry.

In accordance with dipole selection rules, the $^4I_{13/2} \rightarrow {}^4I_{15/2}$ transition is forbidden, so Er^{3+} in the free space doesn't give 1.54μm luminescence. When the Er^{3+} is on a site of tetrahedral symmetry, the crystal-field caused by the surrounding atoms will split the 16-fold degenerated ground state $^4I_{15/2}$ into three four-fold states Γ_8 and two doublet states Γ_6 and Γ_7. Correspondingly, the 14-fold degenerated excited state $^4I_{13/2}$ is splitted into two Γ_6, one Γ_7 and two Γ_8 states, where Γ_6, Γ_7 and Γ_8 are additional irreducible representations of the double group of Td , the tetrahedral group. The dipole transforms according to Γ_5. We examine the group-theoretical decomposition of the dipole times the possible initial(excited) state representation which are Γ_6, Γ_7 and Γ_8,

$$\Gamma_5 \otimes \Gamma_6 = \Gamma_7 \oplus \Gamma_8,$$
$$\Gamma_5 \otimes \Gamma_7 = \Gamma_6 \oplus \Gamma_8,$$
$$\Gamma_5 \otimes \Gamma_8 = \Gamma_6 \oplus \Gamma_7 \oplus 2\Gamma_8,$$

the $\Gamma_6 \rightarrow \Gamma_6$ luminescence would be forbidden if the excited state were Γ_6; the $\Gamma_7 \rightarrow \Gamma_7$ transition would be forbidden if the initial state were Γ_7, and the other dipole transitions are allowed.

3 Luminescence Spectra and Discussion

The silicon substrate of n tpye, (100) orientation was used, after standard clearing process, the sample was implanted with Er ions with the energy of 300keV, and the dose of $5\times10^{13}cm^{-2}$, then annealed at 650℃ for 2 hours and at 900℃ for 2 minutes in order to

recover the lattice damages and make Er^{3+} to be optically active. PL measurements were made by using the standard phase-locked system and the sample was mounted in the cryosystem getting the temperature of about 10K. The measured PL spectrum is given in Fig. 2. Nine luminescence lines are found in PL spectrum of Si : Er. Besides the main line at 1.54μm , there are eight weaker lines at lower energy side. The wavelengths and wavenumbers of nine lines are shown in Table 1. The comparably stronger lines α_1, α_2, α_3, α_4 and α_5 at 1.536μm, 1.554μm, 1.574μm, 1.597μm and 1.64μm respectively are attributed to the transition from the lowest-energy splitting level α of $^4I_{13/2}$ to five splitting levels of $^4I_{15/2}$. The rest four lines β_2, β_3, β_4 and β_5 at 1.547μm, 1.567μm, 1.591μm and 1.634μm locate at the high energy side of corresponding α lines, respectively. The energy separation between these emission lines are 25cm^{-1}, 25cm^{-1}, 23cm^{-1} and 26cm^{-1}, with the deviation being less than 3cm^{-1}, which are within the resolution limit in our equipment. So we think that β_2, β_3, β_4 and β_5 lines are contributed from the transition starting from the second lowest splitting state β of $^4I_{13/2}$. The energy splitting between α and β states is about 25cm^{-1}.

Table 1 The spectrum lines of Er ion in silicon

	α_1	β_2	α_2	β_3	α_3	β_4	α_4	β_5	α_5
wavelength/μm	1.536	1.548	1.544	1.567	1.573	1.591	1.597	1.634	1.641
wavenumber/cm^{-1}	6510	6460	6435	6382	6357	6285	6262	6120	6094

The spectrum given in Fig. 2 is compared with other published results, showing the similalities are striking. For example, the five spectral lines were reported by Tang *et al.*[6], especially the line positions are very similar to five α_i lines in Fig. 2. Tang also attributed these lines to the crystal-field splitting of Td symmetry. Frederick *et al.*[7] reported the spectra of Er^{3+} in silicon and figured out five lines similar to those shown in Fig. 2. But they both assigned the lowest-energy splitting state α in the $^4I_{13/2}$ manifold as the doublet degenerated states (Γ_6 *or* Γ_7). We prefer to have different assignments: our explanation for measured luminescent spectrum identifies the lowest excited state α to be Γ_8. According to the mentioned group symmetry theory, if the lowest excited state is Γ_6 or Γ_7, the $\Gamma_6 \rightarrow \Gamma_6$ or $\Gamma_7 \rightarrow \Gamma_7$ luminescence would be forbidden, but if the lowest excited state is Γ_8, all dipole transitions, Γ_8 to Γ_6, to Γ_7, and to Γ_8, are allowed. Hence, only the assignment of the lowest excited state to fourfold degenerated Γ_8 leads to five spectral lines. It is obvious that they neglected the dipole selection rules in Td symmetry resulting in the assignment of α state to the doublet degenerated state(Γ_6 or Γ_7). Only four spectral lines relating to β state, appear in Fig. 2, we think also this is the result of dipole selection rules: the lowest-energy splitting state in $^4I_{15/2}$ is doublet degenerated state (Γ_6 or Γ_7), and the state β in $^4I_{13/2}$ belongs to the same irreducible representation Γ_6 or Γ_7, thus the dipole transition between them is forbidden, the lines β_1 disappears.

PL Spectra(Fig. 3) from Si : Er+O and from Si : Er are compared, they are similar each other: five stronger lines followed with four weaker lines. According to the experi-

ment results we suggest that the luminescence centers both in Si : Er+O, and in Si : Er, have the same symmetry of Td group, meaning that oxygen codopants around Er^{+3} do not reduce the symmetry of the crystal field at Er ion site but increase the transition probabilities for luminescence and hence greatly increase the PL intensity. Meanwhile the $^4I_{13/2} \rightarrow {}^4I_{15/2}$ transitions forbidden in the free space are allowed with the symmetry of Td group except for $\Gamma_6 \rightarrow \Gamma_6$ and $\Gamma_7 \rightarrow \Gamma_7$ transitions. So the symmetry reduction of crystal field at the Er^{3+} site has no much significance.

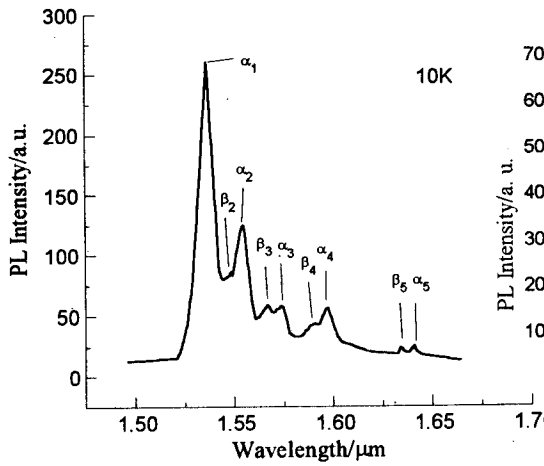

Fig. 2 Spectrum of erbium-doped silicon

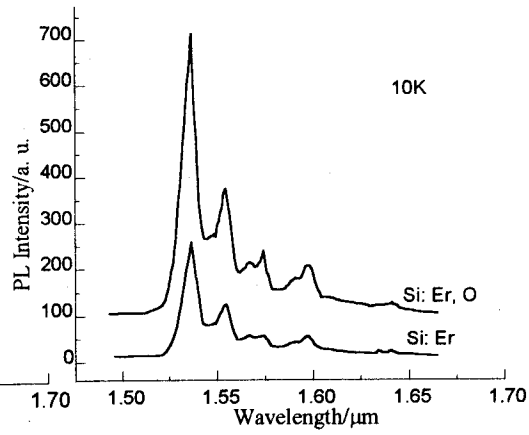

Fig. 3 PL spectra of Si : Er and Si : Er, O

4 Conclusion

The crystal-field splitting model of Er luminescence center with Td symmetry in silicon is presented. Nine luminescence lines are observed in Er-implanted silicon samples and they are attributed to the dipole transition from the lowest-energy (fourfold degenerated state Γ_8) and the second lowest-energy splitting states (doublet degenerated state Γ_6 or Γ_7) to the splitting levels of $^4I_{15/2}$. The oxygen co-implantation greatly increase the PL intensity having the spectra similar to that from the samples without oxygen co-implantation meaning that the oxygens around Er do not reduce the symmetry of crystal field at Er site.

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