

# RBS-CHANNELING ANALYSIS OF ER $\delta$ - DOPED LNP(001) CRYSTAL

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## Abstract

The lattice location of Er  $\delta$ -doped in InP(001) crystal by organometallic vapor phase epitaxy (OMVPE) was carried out by means of Rutherford backscattering spectrometry (RBS) with the channeling technique. The Er yield curve around the  $\langle 001 \rangle$  direction shows a small dip and those around the  $\langle 011 \rangle$  and  $\langle 111 \rangle$  directions show a small flux peak. The flux peak along the  $\langle 111 \rangle$  is lower than that along the  $\langle 011 \rangle$  direction. These data suggest that Er atoms occupy the site equivalent to the hexahedral one in InP lattice.

## 1. Introduction

There has been increasing interest in rare-earth (RE) doped III-V semiconductors for their possible applications to optoelectronic devices [1-3]. Feasibility of near-infrared lightemitting diodes (LED) and semiconductor lasers is based on the observation of the 4f-intrashell emission lines that are characteristic of the dopant, independent of the host crystal, and insensitive to temperature.  $\delta$ -doping of RE in III-V semiconductors with nanoscale quantum structures is an important technique necessary for future device applications.

So far, it has been shown by J. Nakata *et al.* that Er atoms form NaCl-type crystalline ErAs clusters in the GaAs epitaxial layer, based on the analysis of the ion-channeling spectra using a Monte Carlo simulation [4]. It describes that almost all Er atoms are located precisely in the tetrahedral interstitial site to the GaAs lattice. Recently, Erbium (Er)  $\delta$ -doping to InP has been performed successfully by organometallic vapor phase epitaxy (OMVPE) for the first time and characterized systematically by means of X-ray crystal truncation rod (CTR) scattering, photoluminescence (PL), and RBS measurements [5]. X-ray CTR scattering with synchrotron radiation revealed clearly the atomic-scale Er profile in InP. In 4.2 K PL measurements, a characteristic Er-related emission was observed in all the Er  $\delta$ -doped specimens. RBS measurements showed that the Er sheet density was directly proportional to the Er source supply time. Moreover, very recently, the extended X-ray absorption fine structure (EXAFS) analysis of Er  $\delta$ -doped in the InP(001) crystal by OMVPE has shown that Er atoms form NaCl-type crystalline ErP clusters in the InP epitaxial layer [6].

In this paper, the lattice location of Er  $\delta$ -doped in the InP(001) crystal by OMVPE and the crystalline quality of InP overgrown have been studied by means of the RBS channeling technique.

## 2. Experimental

The specimen of Er  $\delta$ -doped InP(001) crystal was prepared by utilizing the low-pressure growth system with a vertical quartz reactor. Details of the growth system were described previously [7]. TMIIn (trimethylindium) and TBP (tertiarybutyl phosphine) were used as source materials for InP growth. Er(MeCp)<sub>3</sub> (tris(methylcyclopentadienyl) erbium) as the Er source was maintained at 100°C and introduced in the reactor by H<sub>2</sub> flow through the cylinder. The sequence of the  $\delta$ -doping of Er in InP, shown schematically in Fig.1, was as follows: I) The InP buffer layer of 1000 Å in thickness was grown on a (001)-oriented Fe-doped InP substrate at 530<sup>0</sup> C. 2)

The supply of TMI<sub>n</sub> was stopped to suspend the growth. 3) The Er source was supplied at the growth temperature to form an atomic plane of the dopant on the surface. 4) After the supply of the Er source was stopped, a purge period of 30 s was inserted to ensure the gas change. 5) The InP cap layer of 50 Å in thickness was grown on a InP (001) substrate at 530°C. TBP was flowed continuously during a series of steps. The exposure duration to the Er source was 80 min.

The RBS-channeling measurements were carried out in another UHV chamber that was connected to a beam line of a 2 MeV Van de Graaff accelerator. The specimen with a size of 10x8x0,35 mm<sup>3</sup> was mounted on a three-axes rotatable goniometer with two-axes linear motion having an angular resolution of 0,025° and a well-collimated (<0,01°) 1.8 MeV He<sup>+</sup> beam of 1 mm in diameter was irradiated to the sample. The backscattered He<sup>+</sup> ions were detected with a silicon surface barrier (SSB) detector at scattering angles of 153° and 99°, with an energy resolution of 13 keV full width at half maximum (FWHM). The beam current was measured with a bias of +90 V supplied to the sample in order to suppress the secondary electron emission. The beam current was typically 2 nA and a total He<sup>+</sup> ion fluence to obtain one RBS spectrum was 3x10<sup>15</sup> ions/cm<sup>2</sup>. Angular scans of the backscattering yield were done around the <001>, <011>, and <111> directions. In the <001> aligned RBS-channeling measurements, the scattered He<sup>+</sup> ions were detected at the angle of 99° in addition to 153°, in order to evaluate the crystalline quality of InP cap layer with the high depth-resolution. Relatively high depth-resolution of 32 Å is achieved in detection at the angle of 99° (low scattering angle condition).

### 3. Experimental results

Typical RBS spectra of He<sup>+</sup> ions backscattered from the Er δ-doped InP (001) substrate to the scattering angles of 153° and 99° are shown in Figs.2 (a) and 2 (b), respectively, where open and closed circles represent the random and the <001>-aligned spectra, respectively. From the ratio of the aligned to the random yield at the scattering angles of 153° and 99°, it was estimated that the average minimum yields  $\chi_{\min}$  in different depths marked by the arrow were 4,3 % and 2,2%, respectively. The concentration of Er δ-doped in the InP(001) crystal was estimated from both spectra at 153° and 99° to be 1,9x10<sup>15</sup> cm<sup>-2</sup> and 2,1x10<sup>15</sup>cm<sup>-2</sup>, respectively. Er yields at the channeling spectrum is almost the same as those at the random spectrum, which indicates that Er atoms are not located in the tetrahedral sites. It is also seen that In surface peak in Fig.2 (b) has a tailing to a lower energy side than the surface peak. The value of  $\chi_{\min}$  in the depths corresponding to the cap layer was 15%.

In order to determine the lattice site of Er δ-doped in the InP(001) crystal, the angular scans of the scattering yields from Er and In atoms were measured around the <001>, <011>, and <111> directions. Typical RBS spectra of He<sup>+</sup> ion backscattered from the Er δ-doped InP(001) substrate are shown in Fig.3, where open circle and closed and open triangles represent the spectra of the <011> aligned and +0,95° and -1,05° tilted from the <011> aligned direction, respectively. The Er and In normalized yields are shown in the <001>, <011>, and <111> directions in Fig.4. The In normalized yields were obtained from the total counts in the window width between 350 and 370 channels, shown in Fig.3.

### 4. Discussion

From the RBS-channeling spectra in the <001> direction, as shown in Fig.2, it is seen that the values of  $\chi_{\min}$  for the InP at the scattering angles of 153° and 99° are 4,3 % and 2,2 %. The depths marked by the arrows are corresponding to the substrate and buffer layer, respectively. This fact indicates that the crystalline quality of the buffer layer is excellent and the buffer layer is coherent with InP substrate. On the other hand, In surface peak in Fig.2 (b) has a

tailing to a lower energy side than the surface peak. This region is corresponding to the cap layer. The value of  $\chi_{\min}$  (15 %) indicates that the crystalline quality of the cap layer is a little bit poorer than that of the buffer layer.

It is seen, according to the eye guide line in Fig.4, that the Er yield curve around the  $\langle 001 \rangle$  direction shows a small dip. The narrow peaks of Er are observed in the directions of  $\langle 011 \rangle$  and  $\langle 111 \rangle$ , which can be attributed to the flux-peaking effect, except that the angular profile in the  $\langle 011 \rangle$  direction is somewhat asymmetric, which is discussed later. The flux peak along the  $\langle 111 \rangle$  direction is lower than that along the  $\langle 011 \rangle$  direction. Although the angular dependence of In yields shows somewhat planar-channeling effect at negatively large tilt angles to the  $\langle 111 \rangle$  direction, as shown in Fig.4 (c), the angular profile at small tilt angles near the  $\langle 111 \rangle$  direction is independent of the fact. Therefore, these angular profiles indicate that Er atoms are not shadowed by the In atomic rows in the three directions of InP crystal. If Er is situated at the tetrahedral site, Er atoms are completely shadowed by the In atomic rows in the  $\langle 001 \rangle$  and  $\langle 111 \rangle$  directions. Thus, the present experimental results are concluded to rule out the tetrahedral site for Er atoms.

So far, in order to determine the impurity location from the angular profile of the backscattering yield, the yield profiles for different interstitial sites have been calculated by K.Morita using the Monte Carlo simulation [8]. According to his calculation, the yield profiles for the hexahedral interstitial site in Si crystal show so-called off-axis peaks, likely a small dip in the  $\langle 001 \rangle$  direction, a clear flux peak in the  $\langle 011 \rangle$  direction and a small flux peak in the  $\langle 111 \rangle$  direction. The characteristics of these yield profiles for the hexahedral sites in Si crystal are qualitatively consistent with those of the present experimental ones. The atomic row structures in the III-IV cubic ZnS type lattice of InP are different from that in diamond lattice of Si. However, the flux distribution of channeled ions at small tilt angles to the channeling direction in the former lattice is expected to be almost the same as that in the latter lattice. Therefore, the present yield profiles in three channeling directions may be concluded to indicate that Er atoms are situated in the site equivalent to the hexahedral site of diamond lattice, which are schematically shown in Fig.5, where large circles represent four equivalent Er positions projected onto the planes in perpendicular to the three directions of InP lattice. It is seen from Fig.5 that the  $\langle 111 \rangle$  atomic row structure of InP is the same as that of Si, while the atomic row structure in the  $\langle 011 \rangle$  (or  $\langle 001 \rangle$ ) direction of InP is composed of two  $\langle 011 \rangle$  (or  $\langle 001 \rangle$ ) atomic row structures of face-centered-cubic P and In lattice. Since the atomic numbers of P and In are 15 and 49, respectively, the tilt angle of the  $\text{He}^+$  ion beam, below which the flux distribution of channeled ions in InP lattice is regarded to be almost the same as that in diamond lattice, is roughly predicted to be the channeling critical angle ( $0,6^\circ$  for  $\langle 001 \rangle$  and  $0,7^\circ$  for  $\langle 011 \rangle$  from Fig.4(a) and (b)) multiplied by  $(15/49)^{1/2}$ . Since the angular widths of the small dip in the  $\langle 001 \rangle$  direction and the peak in the  $\langle 011 \rangle$  direction are smaller than the critical tilt angles described above, the conclusion that Er atoms are situated in the equivalent hexahedral sites is reasonable.

In the angular profile in the  $\langle 011 \rangle$  direction, the asymmetry that the yields at tilt angles between  $-0,5^\circ$  and  $-1,0^\circ$  are considerably higher than those between  $0,5^\circ$  and  $1,0^\circ$  has been observed. The other clear asymmetry appears in the RBS spectra of Fig.3, where at a tilt angle of  $0,95^\circ$  a prominent peak yield occurs in the subsurface layers while at a tilt angle of  $-1,05^\circ$  a small peak appears in the deeper layers. Such an asymmetric scattering yield is ascribed to the geometrical property of the  $\langle 011 \rangle$  atomic row structure including only one mirror plane (see Fig.5) and the flux oscillation of channeled ions in depths. The prominent peak in the subsurface layers at  $0,95^\circ$  is attributed to focussing effect of channeled ions to the In atomic row. Other details for the asymmetric flux distribution will be published elsewhere [9].

Recently, the extended X-ray absorption fine structure (EXAFS) analysis of the Er atoms  $\delta$ -doped in the InP(001) crystal by OMVPE has shown that the nearest neighbor element to

erbium is phosphorus and the coordination number of erbium is 6 [6]. This result indicates that a NaCl-type ErP lattice is formed in the InP lattice. On the other hand, the above-described RBS-channeling data indicate that the position of Er atoms projected onto the InP lattice is not the tetrahedral site. These facts indicate that the ErP lattice is not matched with the InP lattice at the interface, which is ascribed to the difference between the coordination numbers of P in ErP and InP. From both the EXAFS and RBS-channeling results, it is expected that the ErP(001) small clusters might swerve zigzag about 1.0Å along the (111) plane at the interface on the InP(001) substrate. The present experimental result on the Er  $\delta$ -doped InP(001) is not accordance with that on the Er doped GaAs by Nakata *et al.* [4]. The discrepancy is explained in terms of thickness of doped Er layer. For the thick doped layer, most of channeled He<sup>+</sup> ions, which pass through the cap layer at a channeling state, can also pass through the epitaxial layer at a channeling state, although a small part are dechanneled at the incoherent interface. Under such a condition, the position of Er atoms is equivalent to the octahedral site in face-centered cubic As lattice, which shows the angular profiles very similar to those for the tetrahedral site in diamond lattice. (GaAs is equivalent to Ge for ion-channeling.)

In the case of molecular beam epitaxy on the (111) plane, InP is formed by stacking the layers of A(In) A(P) B(In) B(P) C(In) C(P) A(In) A(P)..... and ErP by staking the layers of A(Er) B(P) C(Er) A(P) B(Er) C(P).....; thus the hetero-interface of InP and ErP should be formed by stacking of single element layers of In, P, and Er. However, the relative positions of In and Er to P should be different from those in InP and ErP because the coordination numbers of P in both lattice are different. The difference between the coordination numbers is relaxed by lateral and vertical deviation of the positions of In and Er relative to P. In the case lateral deviation is expected to be more effective for the relaxation. Such a relaxation may produce layer by layer growth of ErP(111) on InP(111).

## 5. Conclusion

The lattice location and the crystalline quality of Er  $\delta$ -doped in the InP(001) crystal by OMVPE have been studied from the RBS channeling measurements in the directions of <001>, <011> and <111>. The crystalline quality of the buffer layer is excellent and the buffer layer is coherent with InP substrate, while the crystalline quality of cap layer is a little bit poor compared with the buffer layer. The Er yield curve around the <001> direction shows a small dip and those around the <011> and <111> directions show a small flux peak. The flux peak along the <111> is lower than that along the <011> direction. These data suggest that Er atoms occupy the site equivalent to the hexahedral one in InP lattice.

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### Figure Captions

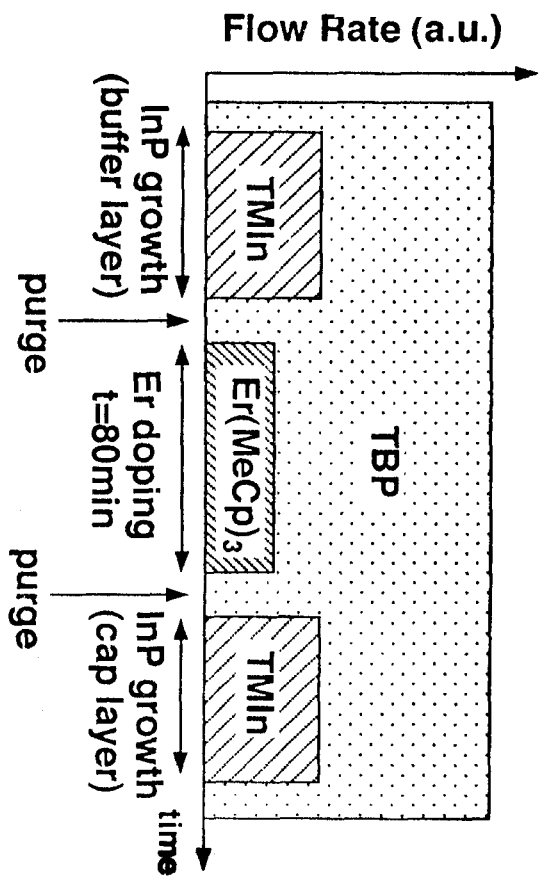
Fig.1. Time sequence of source gases for the  $\delta$ -doping of Er in InP crystal.

Fig.2. RBS spectra of 1,8 MeV He<sup>+</sup> ions from the Er  $\delta$ -doped InP(001) substrate: (○) for random direction and (●) for the  $\langle 001 \rangle$  channeled incidence on the InP substrate measured at the scattering angles of 153° (a) and 99° (b).

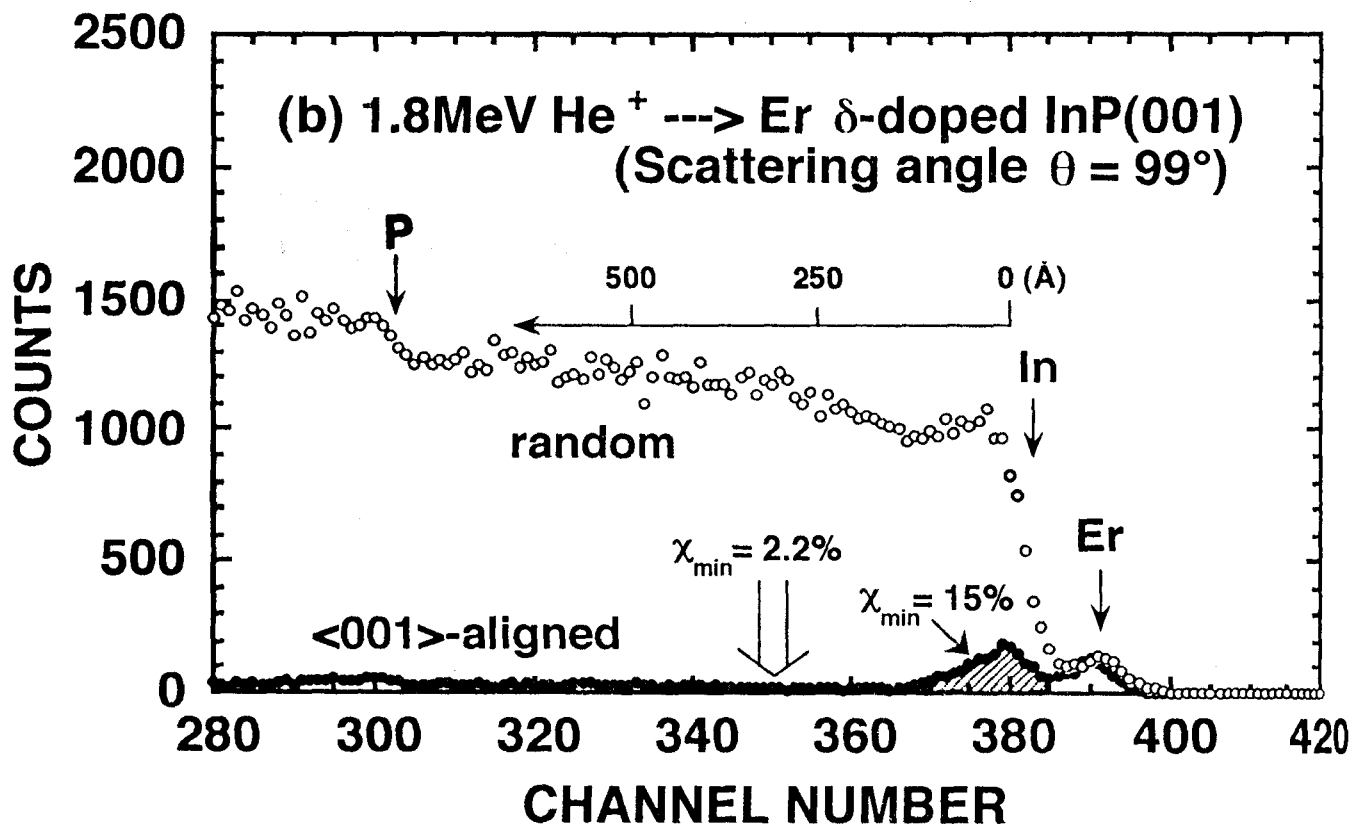
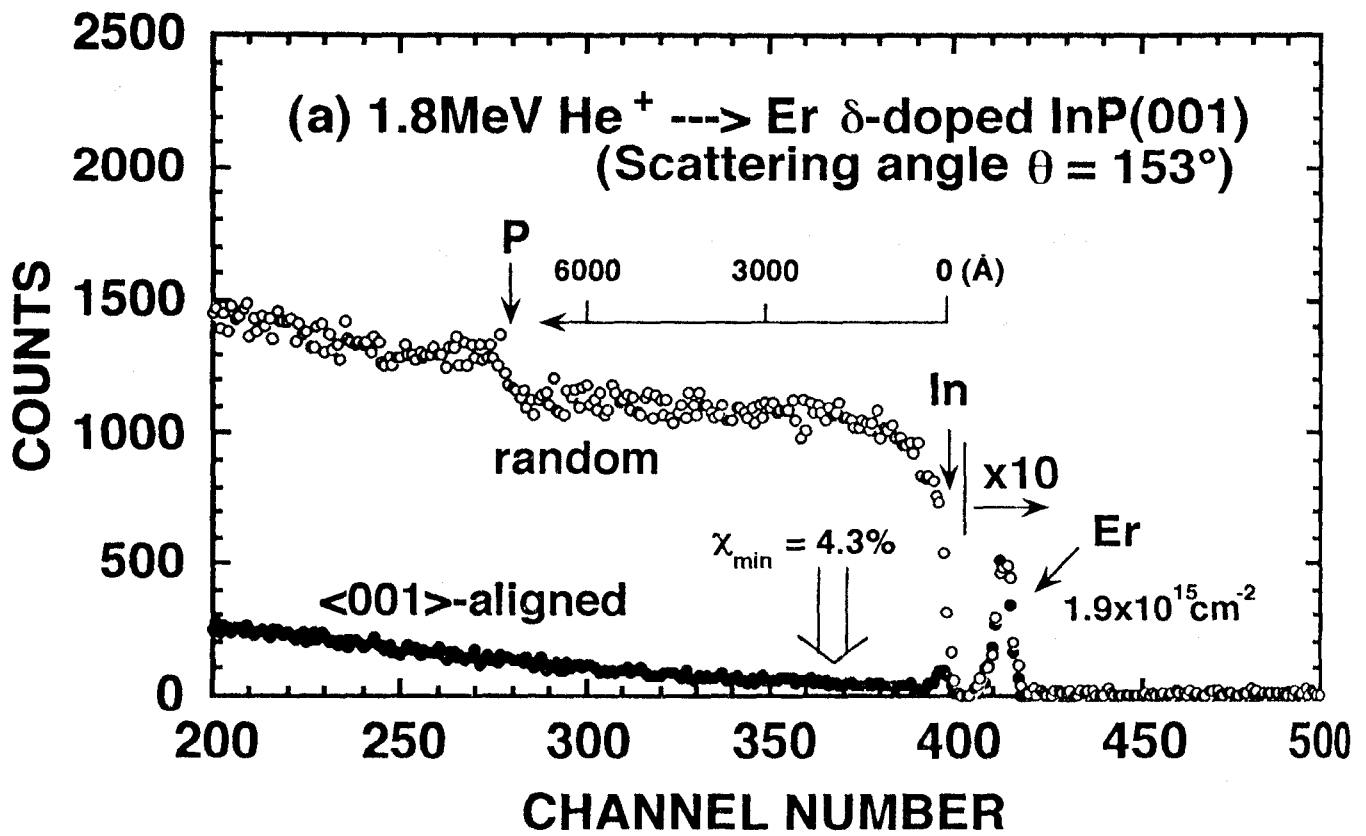
Fig.3. RBS spectra of 1,8 MeV He<sup>+</sup> ions from the Er  $\delta$ -doped InP(001) substrate at the  $\langle 001 \rangle$  aligned (○) and + 0,95° ( $\Delta$ ) and -1,05° ( $\Delta$ ) rotation from the  $\langle 011 \rangle$  aligned direction of the InP(001) substrate.

Fig.4. The angular scans of the backscattering yield of 1,8 MeV He<sup>+</sup> ions from the Er  $\delta$ -doped InP(001) substrate: ( $\Delta$ ) from the Er atoms and (●) from the In atoms, obtained around in the  $\langle 001 \rangle$  (a),  $\langle 011 \rangle$  (b), and  $\langle 111 \rangle$  directions (c).

Fig.5. Projections of the interstitial positions onto the planes transverse to the RBS-channeling direction  $\langle 111 \rangle$ ,  $\langle 001 \rangle$  and  $\langle 011 \rangle$ . The typical hexahedral interstitial sites are shown, which is equivalent to the proposed Er positions.



**Fig.1 J.Yuhara et al.**



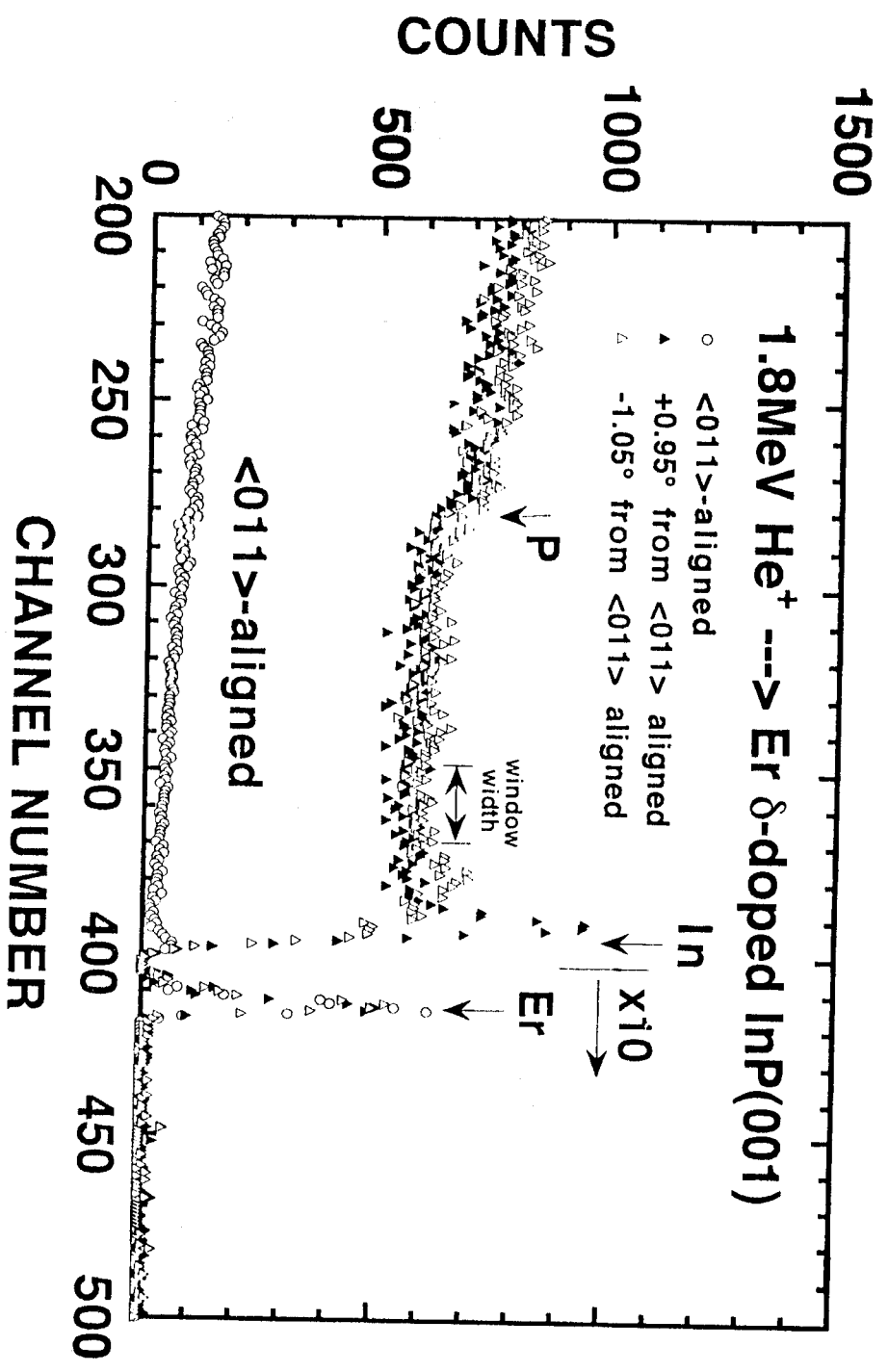


Fig.3 J.Yuhara et al.



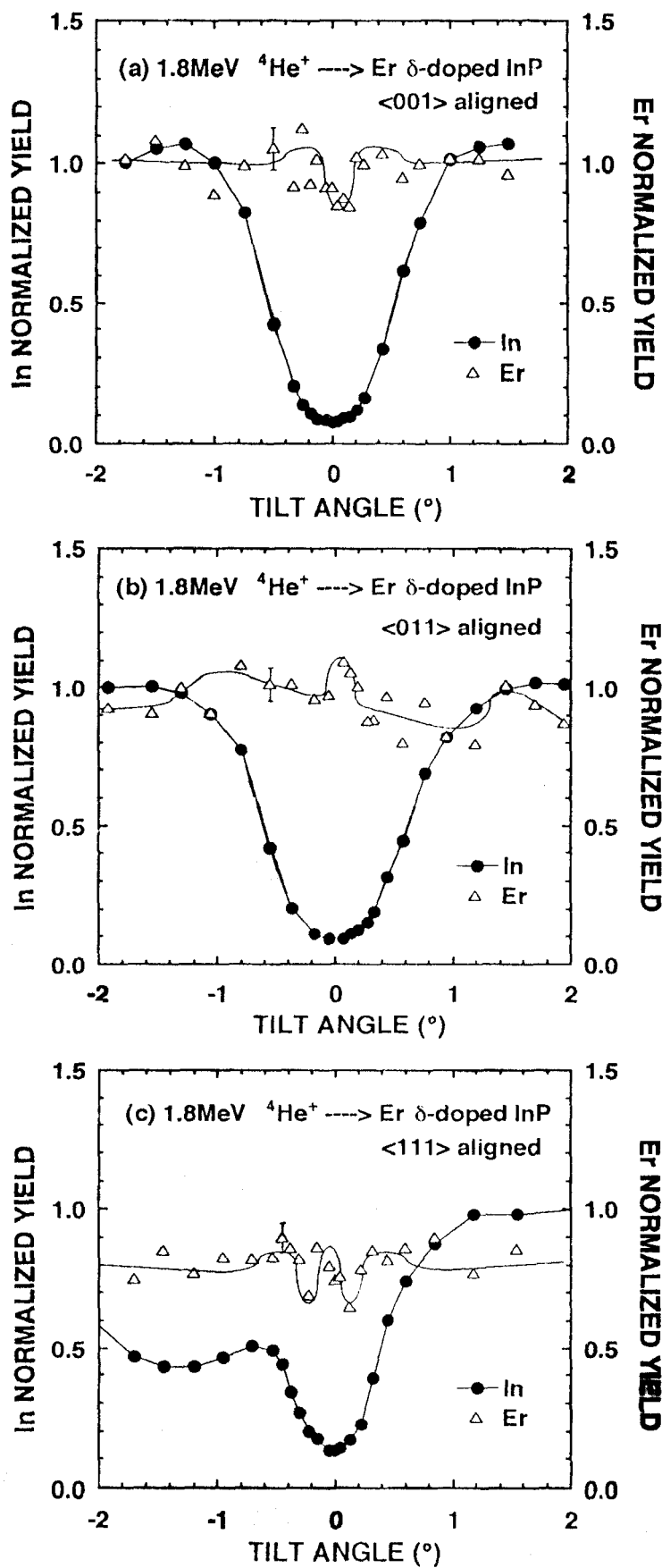


Fig.4 J.Yuhara et al.

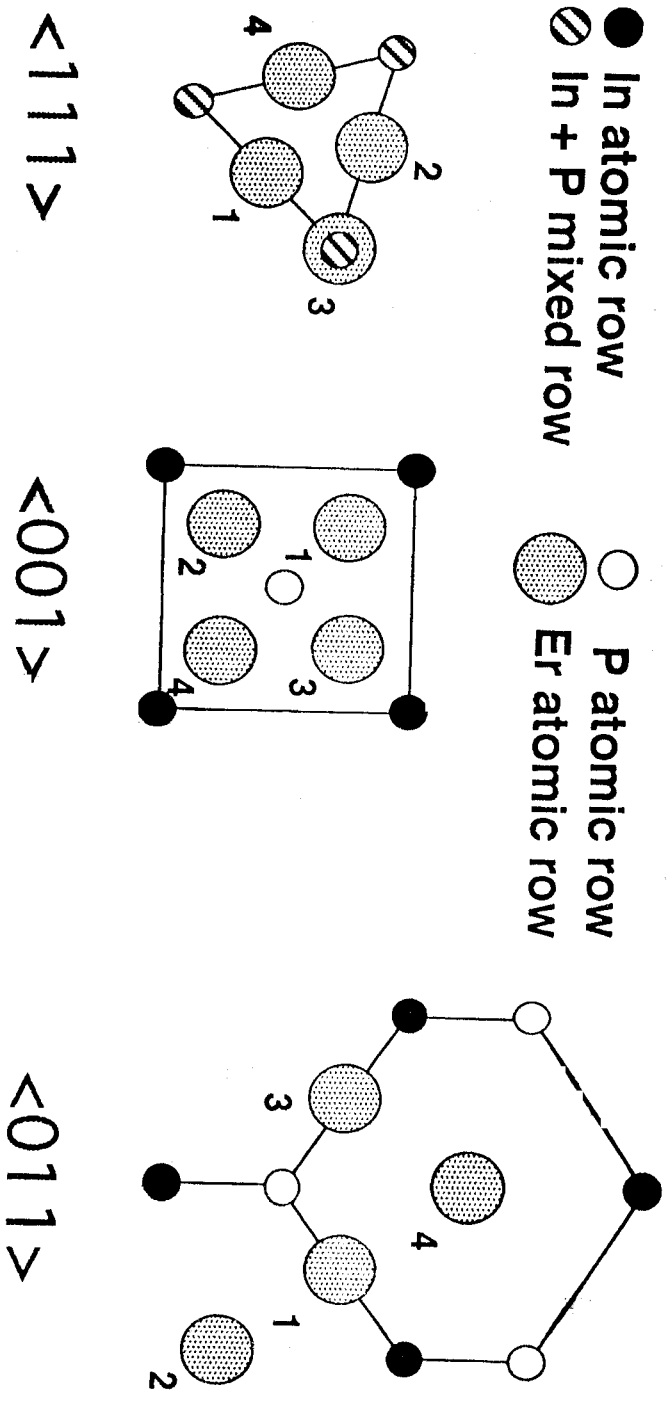


Fig.5 J.Yuhara et al.