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Optical characterization of isolated Se(g)-type misfit dislocations and their influence on strain relief in thin ZnSe films

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Abstract. Microscopic information on the optical properties of Se(g)-type dislocations in ZnSe layers grown on (001) GaAs substrates by molecular beam epitaxy (MBE) have been obtained by using micro-cathodo- and photoluminescence techniques. Se(g)-type misfit dislocations are found to nucleate first in high quality pseudomorphic films above the critical thickness. The individual Se(g) misfit segments are evidenced as the only local emission centres of the so-called Y luminescence. The latter is found to be strongly polarized in the defect line direction and exhibits a pronounced spectrum fine structure, which is related to the particular structural configuration, as determined by the dissociation of perfect 60° dislocation segments into pairs of 30°/90° Shockley partials bordering a stacking fault ribbon.

Studying the dislocation induced Y luminescence with respect to polarization properties and correlation with defect structure yields essential arguments supporting the idea that the dislocation-induced luminescence may be ascribed to 1D excitonic states at the line defect.

The local strain field believed to be origin of defect bound electronic states could be examined at isolated Se(g) dislocations by analysing the microscopic dependence of observed polarization of the free exciton emission in the layer matrix. The polarization properties of free exciton emission results from anisotropic relief of layer strain by the Se(g) misfit segment arrangement.

1. Introduction

Monocrystalline ZnSe is one of the compound semiconductor materials in which glide dislocations exhibit pronounced intrinsic defect induced luminescence, first reported as Y luminescence by Dean [1]. A detailed analysis of the optical properties of the Y luminescence and their relationship to defect structure can provide essential information about the nature of the defect bound electronic state. Glide dislocations are involved in the plastic relaxation process of ZnSe based heterostructures and have an important impact on their successful application in optoelectronic devices, e.g. lasers and LEDs. The small lattice misfit of $f = 0.27\%$ in the ZnSe/GaAs(001) heterosystem results in a low density of misfit dislocations. Full strain relief is realized by only a dislocation line density of $D = 5 \times 10^6$ cm^{-2}. Due to differences in the dynamics of Se(g) and Zn(g) dislocation subsystems a clear asymmetric misfit dislocation arrangement can be observed. Isolated Se(g) and Zn(g) misfit dislocations may be resolved using micro-spectroscopic techniques to study the defect arrangement and defect-related local optical properties. Designation of the polar dislocations used here follows the Huenfeld convention. The terms Se(g) and Zn(g) dislocations refer to glide-set dislocations with edge components according to termination of the {111} extra-half plane in unreconstructed core structure by unpaired Se and Zn atoms, respectively.

In the present work the dislocation induced luminescence and the emission of the surrounding crystal matrix are investigated by means of low-temperature photoluminescence (PL), and cathodoluminescence (CL) microscopy and micro-PL (μPL) measurements. Detailed analysis of the local defect-related Y luminescence inclusive polarization properties and spectrum fine structure is reported. The correlation between the spectroscopic data for Y luminescence and structural configuration of the Se(g) dislocation, is discussed.

Strain induced polarization of the matrix emission is shown to correspond locally to the presence of Se(g) misfit dislocation segments. The polarization property and obtained spectroscopic parameters of the measured spectra suggest that the electronic states at the Se(g) dislocation line are one dimensional in nature [2].

2. Experiment

The sample under investigation was a 165 nm thick ZnSe layer grown by molecular-beam epitaxy on high quality GaAs(001) substrate.

The sample was investigated by high resolution CL microscopy by means of scanning electron microscope (SEM) utilizing panchromatic CL imaging and application of the CL-wavelength imaging technique.

For PL measurement, the samples were immersed in liquid helium at 2 K and optically excited with an Ar^+ ion laser at 3.5 eV.

Low temperature (4 K) μPL measurements were performed under the condition of an excitation at 3.0 eV using a Kr^+ ion laser.

A linear polarizer was used to analyse the polarization of the luminescence in the PL measurements. Special care was taken to ensure that polarization effects of the monochromator grating and excitation source were eliminated.

3. Results

In recent studies [3] a complex plastic relaxation mechanism for MBE-grown ZnSe/GaAs(001) heterostructures in dependence on layer thickness has been established. At the beginning of the plastic relaxation process, Se(g)-type dislocations form preferentially in the ZnSe(001) films just above the critical layer thickness, theoretically determined to be $d_c = 135$ nm [4].

The panchromatic CL map of Se(g) misfit dislocations for a 165 nm epitaxial layer is displayed in figure 1. The CL defect contrasts lines show a mean density $D = 2 \times 10^3$ cm^{-2} and align strictly in the $[1\bar{1}0]$ direction, according to the misfit defect arrangement of the Se(g) subsystem. The CL emission is revealed to be dominantly along the $[1\bar{1}0]$ Se(g) misfit segments. These misfit segments are active radiative recombination centres. The defect-related panchromatic signal is found to exceed the matrix emission intensity by almost one order of magnitude, shown by the intensity profile.

The low energy spectrum displayed in figure 2 represents the Y luminescence and its first LO phonon replica as originating from the Se(g) dislocation segments. A low Hyang-Rhys factor of $S = 0.1$ is determined. The Y emission line has its maximum intensity at 2.612 eV and proves to be strongly polarized. Spectroscopic properties of Y luminescence have been reported in detail first by Worschech *et al* [5]. The maximum intensity $I_{\langle 1\bar{1}0\rangle}$ is observed for polarization along $E_Y \parallel [1\bar{1}0]$ parallel to the contrast line direction. The observed degree of

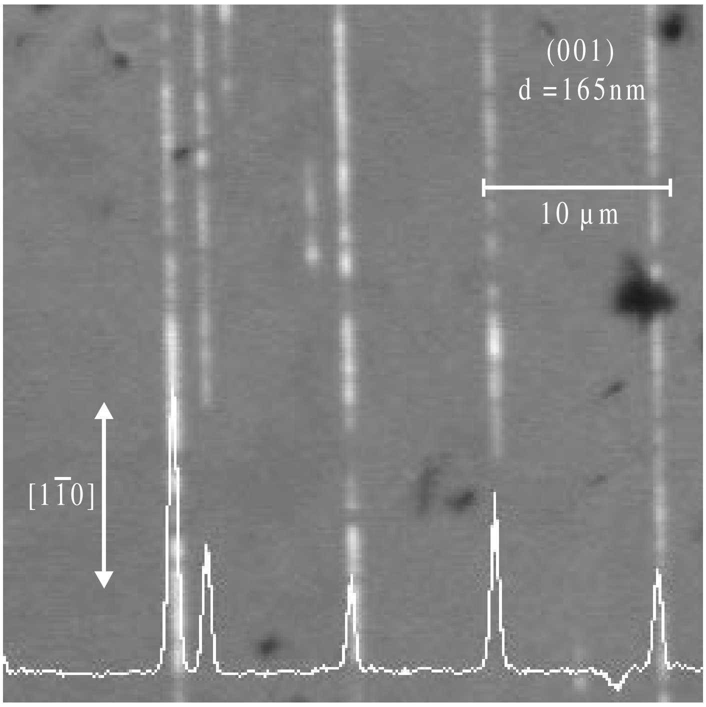

Figure 1. Panchromatic SEM-CL (10 kV, 10 K) micrograph on a ZnSe/GaAs(001) sample reveals bright CL defect contrasts at Se(g)-type misfit dislocations. The defects are radiative radiation centres as evidenced by the CL intensity profile given.

linear polarization defined by

$$\mathrm{DLP} = \frac{I_{\langle 1\bar{1}0\rangle} - I_{\langle 110\rangle}}{I_{\langle 1\bar{1}0\rangle} + I_{\langle 110\rangle}}$$

reaches up to 85%. In the Y luminescence in figure 2 besides the main peak at 2.612 eV additional weaker side peaks can be recognized at the high and low energy side as well. This fine structure of the Y spectrum appears to be of a serial nature as first shown by Worschech *et al* [6]. The Y luminescence peak series has been explained by a model based on the assumption of 60° Se(g) dislocation segments to be dissociated into 30 and 90° Shockley partials. Nucleation of dissociated Se(g) misfit dislocations has also been verified by TEM examinations of ZnSe/GaAs(001) heterostructures [7].

The high energy PL spectrum shown in figure 2 is dominated by the recombination of the free and donor-bound exciton. The lines are split into heavy and light hole components due to lifting of degeneracy of valence bands as caused by a biaxial compressed strained layer. The background emission of the lattice matrix is also polarized, but perpendicular to the Y luminescence. The polarization $E_{xhh} \perp [1\bar{1}0]$ of free exciton emission has its reason in the asymmetry of the long range strain field, produced by the clear asymmetrical misfit dislocation configuration. The dislocation-induced anisotropic strain relief superimposes the initially symmetric in-plane layer stress thus leading to an anisotropic relaxation of the layer matrix.

Figure 3 shows a CL micrograph, in which the contrast of Se(g) dislocations are displayed in wavelength imaging mode. This means, that spatial regions of same recombination energy

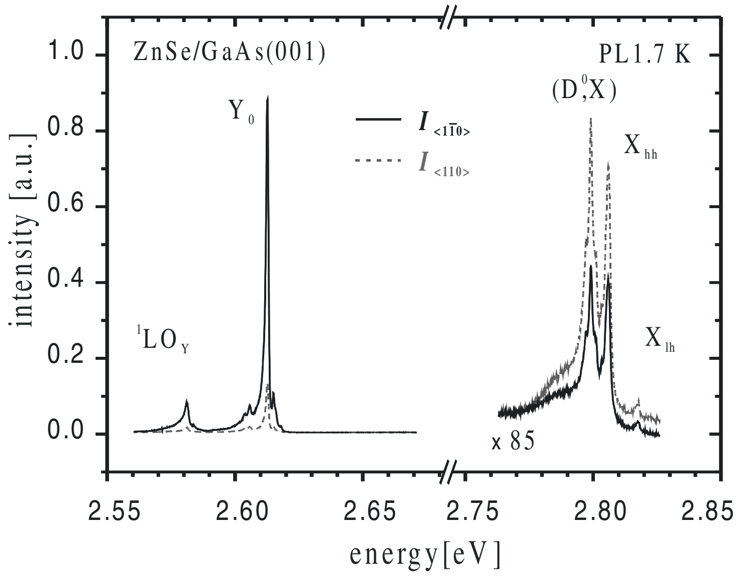

Figure 2. Polarization-dependent PL spectrum from the ZnSe/GaAs sample. Both emission from the layer matrix ($X_{hh,lh}$, D^0X) and defect-induced luminescence (Y_0) show the polarization dependence. However their polarization character is different: Y luminescence is dominant along $E \parallel [1\bar{1}0]$, whereas the free exciton emission is dominant along $E \parallel [110]$.

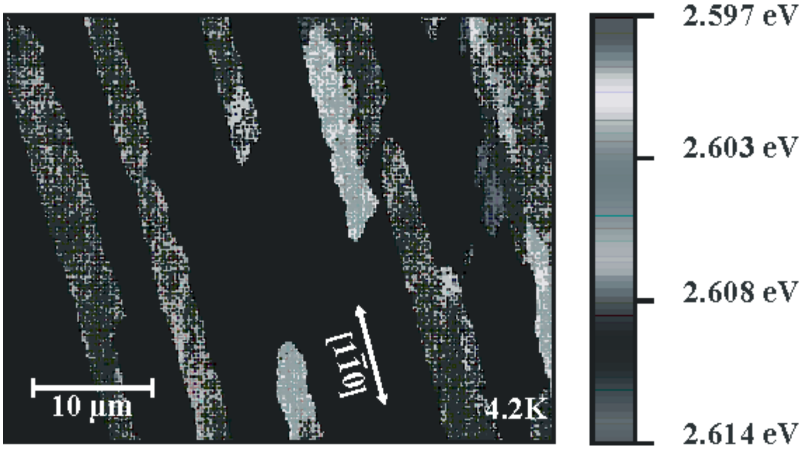

Figure 3. CL contrasts of Se(g) dislocations in the ZnSe(001) epilayer as displayed in wavelength-imaging mode. Cohesive areas with the same level of grey scale represent line segments of distinct width of dissociation into 30 and 90° partial dislocations.

are displayed by the same grey tone. In this imaging mode the line contrasts exhibit a segmentation according to distinct recombination energies along $[1\bar{1}0]$. The image reveal the PL line series to be a superposition, which breaks up into individual spectrum components corresponding to different spatial locations of emission with distinct main peak energies. Following the model proposed in [6] each peak position may be ascribed to a certain dislocation line segment exhibiting specific 30/90° partial dissociation width. This hypothesis seems to be convincingly confirmed by our wavelength imaging studies.

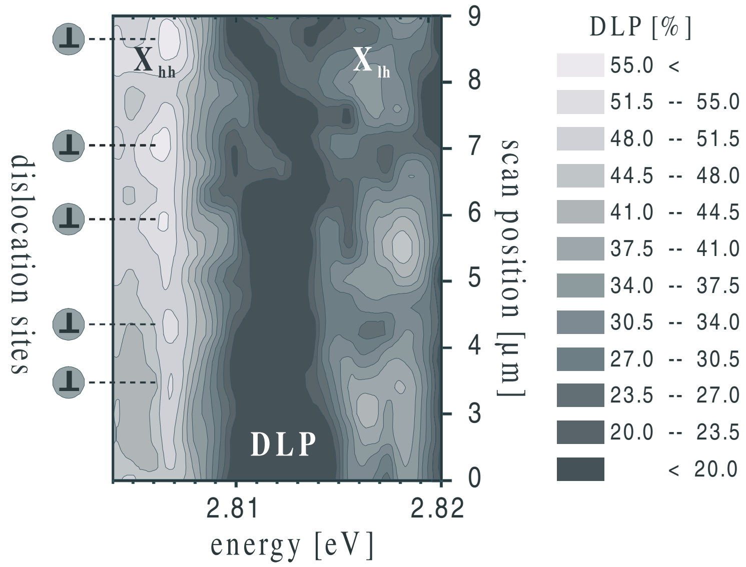

Figure 4. Degree of linear polarization (DLP) of free exciton emission as resolved locally across neighbouring defect lines. Local maximum DLPs of the FX_{hh}, indicating anisotropy of local strain, coincide with positions of Se(g) dislocations.

Analysing the layer matrix emission by polarization-resolved μPL, the particular contribution of isolated Se(g) dislocations to the strain relaxation in the ZnSe epilayer matrix can be revealed.

Therefore two μPL line scans were performed on the same scan path along [110], perpendicular to the dislocation line direction. The PL intensity was recorded for the two polarization orientations. The resulting DLP as a function of photon energy and of the scan path is plotted as a map and shown in figure 4.

It is found, that the DLP of the more intensive X_{hh} line develops the defect positions by coinciding local maximum values. The latter indicate anisotropic local strain relief due to the presence of Se(g) type misfit segments.

Polarization resolved micro-PL measurements in the Y spectral range, which are not included here, demonstrate the occupation of the marked sites by Se(g) dislocation segments. The polarization resolved micro-PL measurement as shown in figure 4 allows us to construct the microscopic distribution of strain field in relation to the local dislocation arrangement.

4. Summary and conclusion

Optical polarization parallel to the dislocation line direction is found for the Se(g) dislocation-induced Y luminescence, as expected by assuming a one dimensional carrier potential [8]. The high value derived for the defect bound exciton energy and the low Hyang-Rhys factor are further support of this model [9, 1]. In this work evidence was given for the inhomogeneous character of the Y luminescence, supporting the model [6] for explaining the fine structure in the spectra.

But considering the recombination activity of A(g)- and B(g)-type dislocations, experiments for CdTe [10] have established similar properties as in ZnSe. This was theoretically worked out by Teichler *et al* [11]. Until now, Te(g) as well as Se(g) dislocations are found to be the radiative recombination centres responsible for Y luminescence. In contrast to this findings the dislocations in the corresponding A(g)-subsystems show defect-induced non-radiative recombination properties.

From these observations we can draw the following conclusions.

Our experimental results clearly demonstrate that the concept of treating dislocations as one dimensional bands holds quite well for describing the optical properties of dislocations in the B(g)-type subsystem. More precisely experimental evidence is given that the 90° partial dislocation is the most favourable candidate for bound exciton states responsible for Y luminescence. Due to the fact that dissociated screw dislocation segments do not exhibit any luminescence, the 30° partial dislocations may be excluded as radiative recombination centres.

By taking into account the strain field only, one is unable to explain the obvious different recombination activity of A(g)- and B(g)-type dislocations in II/VI materials.

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