Defect studies of ZnO films prepared by pulsed laser deposition on various substrates


Introduction

Defect studies of ZnO films prepared by pulsed laser deposition on various substrates

Experimental

• ZnO films were deposited by PLD using a frequency-quadrupled Nd:YAG laser providing 90 mJ of 266 nm laser light in 6 ns pulses at the repetition rate of 10 Hz, ablatting an ultra-high purity ZnO ceramic target with a fluence of target of 2.8 kJ cm⁻². Polished sapphire (0001), MgO (100) and FS substrates baked out in vacuum at 950°C were used for depositions. The ZnO films were grown in an oxygen atmosphere at a pressure of 10 Pa, with a substrate temperature of T=300°C as a result of 5,200 laser shots. A hydrothermally-grown bulk ZnO (0001) single crystal with an O-terminated surface supplied by McTeck GmbH was used as a reference material in SPIS investigations.

XRD studies were performed with an X'Pert MRD diffractometer using CuKα radiation. SPIS investigations were performed using a slow position beam, SPINSOR [7], with the energy of incident positrons adjustable in the range from 0.03 to 36 keV. Doppler broadening (DB) of the annihilation photon peak was measured by a HPGe detector with an energy resolution of (1.09 ± 0.01) keV at 511 keV. Evaluation of DB was carried out using the line shape parameters S and W. The central energy region for the calculation of S was chosen as E – μE₀±0.90 keV and all the S parameters are normalized to the bulk value S₀ = 0.5068(5) determined in the reference ZnO crystal. The energy ranges of 508.21-509.00 keV and 513.00-513.79 keV were used for calculation of the W parameter. All the W parameters were normalized to the reference value of the bulk ZnO crystal W₀ = 0.1039(7).

Figure 1 The dependence of the S (A) and W (B) parameters on the positron energy E for the reference ZnO (0001) single crystal. The mean positron penetration depth zmean is shown on the upper horizontal axis. The solid lines show the model curves calculated by VEPFIT.

Figure 2 Dependence of the S (A) and W (B) parameters on positron energy for bare substrates. The mean positron penetration depth zmean is shown on the upper horizontal axis. The dashed lines show the model curves calculated by VEPFIT for bare substrates.

Figure 3 Dependence of the S (A) and W (B) parameters on positron energy for ZnO films. The mean positron penetration depth zmean is shown on the upper horizontal axis. The dashed and solid lines show the model curves calculated by VEPFIT for bare substrates and ZnO films, respectively.

Table 1 Properties of ZnO films deposited on MgO (100), sapphire (0001) and FS substrates: the film thickness calculated from measurements of optical reflectance and transmittance (tSPIS), determined from XRD reflective curves (tXRD) and estimated by SPIS (tSPIS); the mean crystallite size estimated by XRD (dcryst), the lattice parameters a, c determined by XRD, the lattice parameters S for the ZnO layer (SZnO), the mean positron diffusion length L+ and the surface value of the S parameter (Ssurf / S0).

<table>
<thead>
<tr>
<th>Substrate</th>
<th>MgO (100)</th>
<th>Sapphire (0001)</th>
<th>FS</th>
</tr>
</thead>
<tbody>
<tr>
<td>tXRD (nm)</td>
<td>81(1)</td>
<td>76(1)</td>
<td>76(1)</td>
</tr>
<tr>
<td>tSPIS (nm)</td>
<td>88(6)</td>
<td>81(1)</td>
<td>81(1)</td>
</tr>
<tr>
<td>dcryst (nm)</td>
<td>100(0)</td>
<td>100(0)</td>
<td>100(0)</td>
</tr>
<tr>
<td>a (Å)</td>
<td>0.2495(1)</td>
<td>0.2495(1)</td>
<td>0.2495(1)</td>
</tr>
<tr>
<td>c (Å)</td>
<td>0.507(2)</td>
<td>0.507(2)</td>
<td>0.507(2)</td>
</tr>
<tr>
<td>Ssurf / S0</td>
<td>0.1039(7)</td>
<td>0.1039(7)</td>
<td>0.1039(7)</td>
</tr>
<tr>
<td>L+ (nm)</td>
<td>1.20(2)</td>
<td>1.20(2)</td>
<td>1.20(2)</td>
</tr>
<tr>
<td>Ssurf / S0</td>
<td>1.0566(6)</td>
<td>1.0552(8)</td>
<td>1.06(1)</td>
</tr>
<tr>
<td>E (keV)</td>
<td>1.17(7)</td>
<td>1.18(8)</td>
<td>1.17(6)</td>
</tr>
</tbody>
</table>

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References


Conclusions

• Very thin ZnO films deposited by PLD on various substrates were characterized.

• All films exhibit higher concentrations of open volume defects than a thick ZnO single crystal.

• The ZnO films deposited on the single crystalline substrates (MgO, sapphire) exhibit a higher concentration of defects than film deposited on an amorphous FS substrate. This is most probably due to a higher density of misfit dislocations, which compensate for the lattice mismatch between the film and the substrate.

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