Experiment title: Influence of dopant atoms in cubic boron nitride (c-BN) thin films on lattice parameters and intrisic stress investigated by X-ray diffraction

<table>
<thead>
<tr>
<th>Beamline:</th>
<th>Date of experiment:</th>
<th>Date of report:</th>
</tr>
</thead>
<tbody>
<tr>
<td>BM20</td>
<td>from: 31-Oct-2001 to: 5-Nov-2001</td>
<td>05-Feb-2002</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Shifts:</th>
<th>Local contact(s):</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>N. Schell</td>
</tr>
</tbody>
</table>

Names and affiliations of applicants (* indicates experimentalists):

F. Richter, Th. Peifer, V. Linß, S. Peter*
TU Chemnitz, Institut fuer Physik –123202-, D-09107 Chemnitz, Germany

W. Hoyer, Th. Halm*
TU Chemnitz, Institut fuer Physik –123402-, D-09107 Chemnitz, Germany

Report:

According to our previous experiments, where we investigated thin polycrystalline c-BN films doped with a few at.% aluminium [1], the aim of our last experiment was to investigate the possibility to manipulate the lattice spacing in cubic boron nitride (c-BN) due to the incorporation of the noble gas krypton.

A preliminary study on such c-BN films revealed that the reflex of the (111) lattice planes is well pronounced, therefore, this reflex was chosen to be studied. To obtain a great variety of different orientations of these (111) planes relative to the sample surface, a monochromatic beam of 1.1 Å was used. The angle between the incident beam and the sample surface was fixed at values of 0.3 ° (slightly above the angle of external total reflection).

To access differently oriented planes, the detector was moved either around a horizontal axis (2θ) or a vertical axis (2ω) while the remaining axis was held constant.
The $\sin^2 \Psi$ method (where $\Psi$ is the angle between the vector normal to the lattice plane and the vector normal to the sample surface) was applied to analyze the biaxial stress state. Assuming a reliable value for the c-BN POISSON’s ratio from the literature, the spacing $d_0(111)$ of the unstressed lattice planes was obtained.

We found that, contrary to aluminium incorporation, in the krypton doped films the c-BN (111) unstressed lattice constant $d_0(111)$ does not depend on the krypton concentration. Assuming YOUNGS’s modulus of the bulk c-BN, the biaxial compressive stress value of the films varied in the range between $-11$ and $-20$ GPa at one and the same krypton content. Additional secondary ion mass spectroscopy measurements show that the krypton concentration in the films is independent of the krypton concentration in the process gas. Furthermore the krypton atoms are probably incorporated at interstitial sites and prior into the hexagonal phase. For a better understanding of the influence of dopant atoms on interstitial sites additional experiments are necessary.

![Graph](image_url)

**Fig. 1** Lattice spacing of (111) planes having different orientations with respect to the sample surface: cubic BN layer with incorporated Kr for different process gas mixtures Kr/Ar = 0/100, 50/50 and 75/25.