SUBSTRATE-INDUCED STRAIN
IN EPITAXIAL LEAD CHALCOGENIDES
BY GALVANOMAGNETIC EFFECT
ROTATIONAL DEPENDENCE

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On the example of the PbTe and Pb$_{0.77}$Sn$_{0.23}$Te on BaF$_2$ the possibility
of using the weak magnetic field resistance technique for the evaluation of
mismatch-thermally induced strains in semiconductors with multivalley band
structure is discussed.

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Substrate-induced strain in epitaxial thin films has long been recognized as
a problem which impacts both fundamental studies and applications. Lead chalco-
genides epitaxial films on BaF$_2$ substrates due to their band structure specifics are
a suitable object for investigation because in these semiconductors thermal expan-
sion and lattice mismatched strains break the cubic structure of lattice and lead
to a significant modification of the semiconductor band structure [1, 2]. As it is
shown by Allgaier [3], the distortion degree of band structure and accordingly the
value of elastic strains for n-type PbTe films can be estimated using four-coefficient
weak-field magnetoresistance measurement technique. We extended this technique
for p-type material including samples protected with coatings.

Single-crystal films (up to 5 μm thick) of n- and p-type PbTe and
Pb$_{0.77}$Sn$_{0.23}$Te ($n, p = 5 \times 10^{17} \text{ cm}^{-3}, \mu_n \approx 3 \times 10^4 \text{ and } \mu_p \approx 1.2 \times 10^4 \text{ cm}^2\cdot\text{V}^{-1}\cdot\text{s}^{-1}$
at 77 K) were prepared by the method of flash evaporation in vacuum on freshly
cleaved (111) BaF$_2$ substrates. To measure the Hall coefficient, electrical con-
ductivity and magnetoresistance the standard Hall bar configuration was used.
The samples were etched into their final shape by either photolithographic tech-
niques or grown on a BaF$_2$ substrate through a bimetallic mask. To form the con-
tact pads gold was deposited through masks. Ag wires were soldered to the pads.
with In. Measurements were conducted with a constant current (50 μA) in a con-
stant magnetic field satisfying the condition of weak magnetic field for fixed mobil-
ity of carriers. Rotational dependences were measured by means of rotation of the
sample holder in magnetic field with the 5° spacing. The two experimental config-
urations A and B (i.e. planes of rotation of the magnetic field used in the present
study) are shown in Fig. 1. The magnitude of the weak-field magnetoresistance
(WFMR) is examined in term of the dimensionless coefficients $M^\phi$

$$\frac{\Delta \rho}{\rho_0} = M^\phi (\mu H B)^2,$$

where $\Delta \rho$ is the fractional change in zero-field resistivity $\rho_0$, $\mu H$ and $B$ are the mag-
nitudes of the Hall mobility and magnetic field intensity, respectively. $M^\phi$ depends
on the sample current and magnetic field directions $\phi$ and $\theta$ (Fig. 1). In a cubic crys-
tal, particularly bulk PbTe, $M^\phi$ is completely described by the Seitz–Pearson–Sull
coefficients — $b$, $c$, and $d$. As a result of strain, the symmetry of (111)-oriented
film is reduced from cubic to trigonal. Only one additional parameter is needed to
fully characterize the WFMR in such trigonal crystals — $d'$. 

For two configurations used for rotational WFMR the coefficient $M^\phi$ is given
by

$$M^{\phi A}_\phi = b + \frac{1}{2} c + \frac{1}{3} d + \left(\frac{1}{2} c + \frac{1}{6} d\right) \cos(2\theta_A),$$

$$M^{\phi B}_\phi = b + \frac{1}{4} d - \frac{1}{12} d \cos(2\theta_B) + \frac{1}{6} \sqrt{2} d' \cos(3\phi) \sin(2\theta_B).$$

Equations (2) and (3) are used to extract $b$, $c$, $d$, and $d'$ from the measured
WFMR. We take the value of the parameter $d'$ to be indicative of the strain
induced into the film. When $d = d'$ the strain is absent and the cubic symmetry
remains unchanged.
Substrate-Induced Strain in Epitaxial Lead Chalcogenides...

Fig. 2. Normalized $M_\beta^s$ versus $\theta_B$ in $B$-configuration for the epitaxial layers at 300 K (curve 1) and 77 K (curves 2 and 3) for the samples without BaF$_2$ and with BaF$_2$ evaporated film of 0.5 $\mu$m thickness.

Experiments conducted on a great number of samples demonstrated that at room temperature the deformation is vanishingly small. But after cooling to 77 K a significant change in the form of the orientational dependences occurs, especially for the $B$ configuration (Fig. 2). The most visually impressive form of demonstrating this effect, a pronounced rotation of curve 2 about the initial figure (curve 1), is shown in Fig. 2. It is caused by the strain in the film. This increasing film distortion is ascribed to the thermal-expansion-coefficient difference between the semiconductor film and its BaF$_2$ substrate at low temperature (Table).

<table>
<thead>
<tr>
<th>Material</th>
<th>Lattice constant [nm]</th>
<th>Thermal expansion coefficient [$10^{-6}$/K] at 300 K</th>
<th>at 77 K</th>
</tr>
</thead>
<tbody>
<tr>
<td>PbTe</td>
<td>0.646</td>
<td>19.8</td>
<td>17</td>
</tr>
<tr>
<td>PbSe</td>
<td>0.612</td>
<td>19.4</td>
<td>–</td>
</tr>
<tr>
<td>BaF$_2$</td>
<td>0.620</td>
<td>19.8</td>
<td>7</td>
</tr>
<tr>
<td>Si</td>
<td>0.543</td>
<td>2.6</td>
<td>0.6</td>
</tr>
</tbody>
</table>

TABLE

The main parameters of lead chalcogenides BaF$_2$ and Si.
The value \( d' \) has a significant scatter, but it may be, nevertheless, stated that the samples defined by photolithography possess a significantly lower value of the strain than the samples defined by the mask. Although after repeated cycles between room temperature and 77 K the value of \( d' \) in both cases is equally approaching \( d \). The situation can be explained by extended defect creation [4] because it is accompanied by a charge carriers mobility decrease.

The potentialities of the weak-field magnetoresistance technique are well demonstrated by experiments performed for structures with \( p\)-Pb\(_{0.77}\)Sn\(_{0.23}\)Te epitaxial layer protected by anodic oxide (up to 200 nm thick) or by deposition of BaF\(_2\) (up to 0.5 \( \mu \)m thick). All the measurements were conducted on the samples grown on the same piece of BaF\(_2\) substrate. These samples differed from each other only by the angle \( \phi \). It has been found that while protecting coatings deposition the strain in epitaxial layer at 300 K is not changed within the precision of the experiment. At the same time, as it can be seen in Fig. 2, when for the sample without the BaF\(_2\) layer the angle of turning the rotational dependence \( \Delta\rho \) in the \( B \) configuration after cooling from 300 to 77 K is \( 28 \pm 5^\circ \) (curve 2), then for the sample covered with the BaF\(_2\) film the rotation angle value becomes as high as \( 42 \pm 5^\circ \) (curve 3). It indicates that the tensile strength increases. For anodic oxide the rotational dependences are not changed which is explained satisfactorily by the glassy character of the anodic oxide. Strain relaxation in layers covered with BaF\(_2\) occurs after first few thermal cycles in contrast to the more slower relaxation of the initial samples.

As it has been demonstrated by Zogg et al. [5], low-cost IR sensors may be fabricated on the basis of lead chalcogenide epitaxial layers on Si (111). Table shows that in this case thermal mismatch strains are even more stronger. Thus, it is of a great interest to apply the WFMR technique to study these structures.

References