CALCULATION OF DEFORMATION PARAMETERS OF CaF_2/Si(111) HETEROSTRUCTURES GROWN BY MBE

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Experimental results of the investigation of CaF_2/Si(111) heterostructures, obtained by means of γ-diffractometry [1] were refined in framework of the general dynamical theory of scattering in deformed crystals [2], for the integral reflection coefficient for the γ-ray radiation of the (*hkl*) reflection. R_i^{hkl} is averaged by a dynamical oscillations period, slightness of Bragg angles is taken into account and the term connected with anomalous Borrmann absorption is thrown away [3].

$$R_i^{hkl} = \frac{\lambda}{2\,\Lambda_0^{hkl} \sin 2\,\Theta_B} \cdot \frac{1 - \exp\left(-\frac{\pi}{2\,|B|}\right)}{\pi} \times$$

$$\times \int_{-1}^{1} \frac{\cosh\left\{2\ln\left\{\left[1 + B^2 T^2 (1 - \xi^2)\right]^{1/2} + |B|\, T (1 - \xi^2)^{1/2}\right\}\right\}}{\left[1 + B^2 T^2 (1 - \xi^2)\right]^{1/2}} \cdot \frac{d\xi}{(1 - \xi^2)^{1/2}}. \qquad (1)$$

To account for crystal latttice defects of the initial specimens, on which CaF_2 film was deposited, the renormalization of R_i^{hkl} values were executed. Instead the values of the dynamical integral reflection coefficient the value R_i^{111}, measured at the initial specimen, was used when calculating the strain gradient B by the formula (1) with the purpose of the renormalization of the extinction length of an ideal crystal to the extinction length Λ_0^{hkl} of the real investigated crystal.

Thickness dependence of the strain gradient modulus ($|B|$), accounted by the formula (1), is shown in fig.

The appraisal of the bending radius of the investigated heterostructures was carried out for value $|B|$ by the approximation of the cylindrical bending. Then we have the following dependence between the strain gradient and the bending radius ρ [2]:

$$|B| = \frac{(\Lambda_0^{hkl})^2}{d_{hkl}\,\rho} \cdot \frac{\sin\Psi\,(2 + \nu_{Si})}{2\pi}. \qquad (2)$$

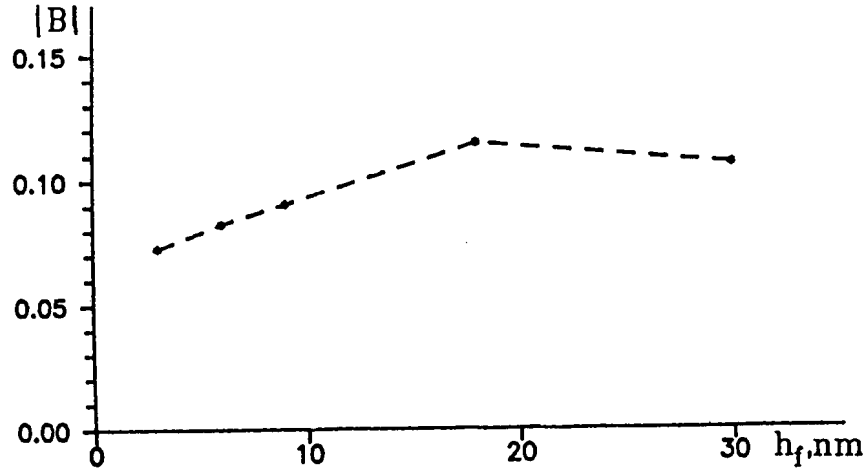

Fig.

The calculated values of ρ are given in table.

Table

Specimen	$h_f(CaF_2)$, *nm*	$R_i^{111} \cdot 10^6$	$\mid B \mid$	ρ, *m*	σ, *Pa*
1	3	8.63 ± 0.04	0.073	1545	$2.18 \cdot 10^9$
2	6	10.64 ± 0.05	0.083	1361	$1.23 \cdot 10^9$
3	9	10.52 ± 0.05	0.091	1240	$9.04 \cdot 10^9$
4	18	13.11 ± 0.09	0.115	982	$5.71 \cdot 10^8$
5	30	12.88 ± 0.06	0.107	1056	$3.17 \cdot 10^8$

We especially comment the possibility of taking very slight bending values of specimens with square $\approx 1\ cm^2$ (kilometer curvature radii).

Carried out investigations show that CaF_2 layers generation on the Si substrate surface resulted in the elastic bending of Si crystals. In the range of the films' thicknesses of 3—18 *nm* values of bending are directly proportional to the CaF_2 layers thickness, and only for the CaF_2 layer with the thickness 30 *nm* linearing of the dependence of strain gradient values from CaF_2 layers thicknesses is broken. At the film-substrate interface of the investigated heterostructures the average meaning of longitudinal stress occurs [4]:

$$\sigma = [\, E_{Si} / 6 (1 - \nu_{Si}) \,] \, (h_s^2 / h_f \rho), \qquad (3)$$

where h_s and h_f are the thicknesses of the substrate and the film, respectively.

If this stress will be closed to the yield strength of the material, the dislocations origin will begin.

According to the formula (3) the calcelations of the stresses value occurring in the film were carried out with the use of the obtained values of the heterostructures bending radius. The data is given in the Table. This appraisal indicates, that the stresses which have occured are close to the yield strength values at the room temperature σ_T (Si) = $7.0 \cdot 10^9\ Pa$ and at high temperatures this stresses may exceed them. Thus with the CaF_2 layers thicknesses more than critical one because of a difference between the thermal expansion coefficients and a misfit of the lattice constants for the film and the substrate the defect formation process in the substrate with the dislocation generation begins.

References

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