11.3-1 INCLUSION-LIKE DEFECTS IN InP SUBSTRATES AND RELATED DEFECTS IN HETEROEPITAXIAL AND Zn-DIFFUSED LAYERS
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InP substrates grown by the liquid encapsulated Czochralski technique often contain typical inclusion-like defects (ILDs), which consist of a central core from which dislocation loops are punched out in the <110> directions. It was previously reported that ILDs affect adversely the epilayer morphology.
In the present work the correlation between ILDs in InP substrates and crystal defects in InGaAs and InGaAsP epilayers and in Zn-diffused InP layers has been studied by X-ray topography and scanning electron microscopy.
Evidence for the propagation of dislocation loops from the substrate into the epilayers has been obtained. More in detail, the dislocation loops lined up along the <110> directions inclined by 45° with respect to the interface have been seen to continue in the epilayers.
In addition to this, ILDs behave as starting points for the emission of misfit dislocations. The origin of these dislocations is of course the misfit strain, which depends on the lattice mismatch and the layer thickness. However, the strong anisotropic stress connected to the ILDs provides a suitable nucleation source for misfit dislocations.
An analogous observation has been made in the case of cracks caused by a heavy Zn diffusion in InP crystals. Once again, the present study has shown that ILDs tend to act as sources of cracks.

11.3-2 CRACKS IN InP-BASED HETEROSTRUCTURES.
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InGaAs/InP and InAlAs/InP single heterostructures grown by molecular beam epitaxy and InGaAsP/InP single heterostructures grown by liquid phase epitaxy under large negative lattice mismatch conditions have been investigated in order to clarify the physical mechanisms of crack formation and propagation. X-ray topography and scanning electron microscopy in the integral cathodoluminescence mode have been mainly employed.
In all cases cracks, generated at the epilayer-substrate interface, propagate into both the epilayer and the substrate. Cracks parallel to the $[1\bar{1}0]$ direction originate at a misfit stress level lower than those parallel to the $[110]$ direction, as demonstrated by the unidirectional crack arrangement along the $[1\bar{1}0]$ direction often observed. Moreover, the cracks parallel to the $[1\bar{1}0]$ direction propagate for larger depths into the substrate than those parallel to the $[110]$ direction.
This asymmetric character of the cracks supports the model for their formation already reported (G.H. Olsen et al., J. Electrochem. Soc. 121, 1651 (1974)). This model assumes that cracks are originated by glide and combination of misfit dislocations. On the other hand, it is well known that α-type dislocations, parallel to the $[1\bar{1}0]$ direction, have a higher mobility than β-type dislocations, parallel to the $[110]$ direction. An analogous behaviour is expected to be exhibited by the cracks, as it has been in fact observed in the present work.

11.4-1 PHASON DISPERSION CURVES IN TANTALUM DISULPHIDE BY X-RAY SCATTERING. By W. Minor, L.D. Chapman, S.N. Ehrlich and R. Colella , Physics Dept., Purdue University, W. Lafayette, Indiana, 47907, U.S.A.

The thermal diffuse x-ray scattering in the neighborhood of first order satellites has been measured with high resolution in $1T_1-TaS_2$ (incommensurate phase), using synchrotron x-rays at NSLS (λ=0.711 Å). A total of about 2400 points in q-space have been measured at 363 and 423 K in small "boxes" surrounding two first order satellites, one close to (010) and the other one close to (030). A preliminary analysis shows that Phason Diffuse Scattering (PDS) falls off like q^{-2}, and that the isodiffusion surfaces surrounding a satellite reflection are ellipsoids, reflecting the anisotropy of PDS as predicted by theory[1]. For a satellite whose projection on the hk0 plane is located along the $\vec{b}^*$ axis, the largest ellipsoidal axis is parallel to $\vec{c}^*$, and the shortest one is parallel to $\vec{b}^*$. The ratios of the three axes are 2.5, 1.8, 1. Absolute measurements of the scattered intensity have led to a quantitative determination of the phason velocities (v_ϕ's) in various directions. The value of v_ϕ along $\vec{b}^*$ is about 1.3×10^5 cm/sec, while along $\vec{c}^*$ the velocity v_ϕ is about 1/3 smaller (4.4×10^4 cm/sec). As the temperature is increased from 363 to 423 K, the velocity along $\vec{b}^*$ is essentially unchanged, but along $\vec{c}^*$ the value of v_ϕ is decreased by 13 % approximately. This work will be the first example of a fully determined phason spectrum.

1) A.W. Overhauser. Phys. Rev. **B 3** , 3173 (1971).

11.4-2 COMPILATION OF TEMPERATURE FACTORS OF CUBIC MATERIALS*. By N.M. Butt, B.T.M. Willis+, G. Heger++ and J. Bashir, Pakistan Institute of Nuclear Science and Technology, Islamabad, Pakistan.

The Temperature Factor is an important parameter in crystal vibration studies. It is related to the magnitude of the amplitude of atomic vibration in a crystal. It is therefore an important parameter of interest in reactor technology and crystal physics.

Several experimental techniques are available for the measurement of this parameter. These are diffraction techniques (x-ray, Mossbauer γ-ray, neutron and electron) neutron scattering techniques, elastic constants, specific heat etc. There is a vast amount of literature which gives values of this parameter determined by various methods. However, in several cubic materials these determinations do not agree with one another. An extensive effort has been made to compile the Temperature Factors of Cubic Materials by various methods, particularly the diffraction methods. An attempt has been made to list the most reliable values available on this parameter for various materials. This paper represents the compilation of temperature factors B and the corresponding mean square atomic amplitudes $\langle U^2 \rangle$ and the Debye temperature H of 22 cubic elements namely, Al, Cr, Cu, Ge, Au, Ir, Fe, Pb, Li, Mo, Ni, Nb, Pd, Pt, K, Rh, Si, Ag, Na, Ta, W and V. Similar data on 70 cubic materials namely, AgBr, AgCl, AgF, AlSb, $AuGa_2$, BaO, $Ba(NO_3)_2$, CaO, CaF_2, CdTe, CeO_2, CsBr, CsCl, CsF, CsI, Cr_3Pt, Cr_3Rh, CuBr, CuCl, EuSe, FeS_2, GaAs, GaP, GaS, GaSb, HfC, HgSe, HgTe, InAs, InP, InSb, KBr, KCl, KF, KI, LiBr, LiCl, LiF, LiI, MgO, Mg_2Si, Mg_2Sn, NaCl, NaBr, NaF, NaI, Nb_3Au, Nb_3P, NH_4Cl, NH_4Br, NiO, $Pb(NO_3)_2$, PbS, PbTe, RbBr, RbCl, RbF, RbI, ReO_3, SiC, SnTi, SrF_2, SrO, $Sr(NO_3)_2$, TiC, TiN, TlBr, TlCl, VO_2, W_2C, ZnS, ZnSe, ZnTe, has been compiled. Recommended values of the Temperature Factors have then been given for the cubic

elements and the cubic materials. This data would be of interest to the solid state Physicists in general and crystallographers in particular.

More data which has not come to the notice of the authors would be welcome for inclusion.

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11.5-1 HIGH-RESOLUTION X-RAY SCATTERING STUDIES OF DEFECT-INDUCED LATTICE DISTORTIONS IN $SrTiO_3$-TYPE PEROVSKITES. By R.J. Nelmes, P.D. Hatton, T.W. Ryan, U.J. Nicholls and H. Vass, Department of Physics, University of Edinburgh, Scotland.

The isomorphous perovskites $SrTiO_3$, $RbCaF_3$ and $KMnF_3$ exhibit the same cubic-to-tetragonal phase transition on cooling through T_c, which is ~100 K for $SrTiO_3$ and ~200 K for the other two. The transition is of the antiferroelectric type. It is almost perfectly second-order in character in $SrTiO_3$, very weakly first-order in $RbCaF_3$ and slightly more so in $KMnF_3$.
We have recently made X-ray scattering measurements of the critical fluctuations in $RbCaF_3$: the results reveal two different length scales above T_c (T.W. Ryan, R.J. Nelmes, R.A. Cowley and A. Gibaud, Phys. Rev. Lett. (1986) 56, 2704). The shorter one is well known: it arises from the usual critical fluctuations and does not diverge at the (first-order) transition. The newly-discovered length scale is much longer, and appears to diverge at T_c. We have suggested that this new feature can be interpreted as arising from large-scale fluctuations into the low-temperature phase (while the sample temperature is above T_c), mediated by the strain energy around defects.
Measurement of the lattice distortion and size of the tetragonal-phase 'clusters' was achieved by determining the displacement and width of the diffraction peaks from the 'clusters' relative to the peaks from the cubic-phase matrix. But the distortion was so small (1 part in 10^4 just above T_c) and the size so large (~2000 Å at T_c + 1 K) that very high reciprocal-space resolution was required. This was achieved by using highly-perfect Si crystals to collimate both the incident and the scattered beams.
Now work on $KMnF_3$ and $SrTiO_3$ has shed new light on the nature of the effect. In particular, we find the cluster size increases in the sequence $KMnF_3 \rightarrow RbCaF_3 \rightarrow SrTiO_3$.

11.5-2 A MONOCHROMATIC BOND METHOD USING SYNCHROTRON RADIATION. By S. Yasuami[1], K. Usuda[1], H. Kawata[2], Y. Higashi[2] and M. Ando[2], 1: R and D Center, Toshiba, Kawasaki 210, Japan, 2: Photon Factory, KEK, Tsukuba, Ibaraki 305, Japan.

A method of absolute lattice parameter measurement, applicable to any single crystals, is under development using monochromatic synchrotron radiation. The system is currently feasible with a few parts of one million in precision in lattice parameter determination. That precision will be good enough to tell, for example, a spatial lattice parameter variation of a GaAs wafer. The system consists of a channel-cut pre energy-selector, a monolithic (+,+) monochromator and a sample axis; the measuring angle region of the 2nd and 3rd axis, which is installed with an encoder of 0.36 arc sec is calibrated by an autocollimator. The whole system is under control of temperature with better than 0.1°C during run. Some applications to characterization of several growth conditions of GaAs crystals will be described in detail.

11.5-3 DIFFUSE NEUTRON SCATTERING ON THE NIOBIUM-DEUTERIUM SYSTEM. By J.C. Osborn and T.J. Hicks, Department of Physics, Monash University, Clayton Vic. Australia.

The low concentration, alpha phase of the niobium-deuterium system is a disordered solution of deuterium in the tetrahedral interstitial sites of the bcc lattice. The displacement field of niobium atoms around a deuterium atom has been studied by diffuse elastic neutron scattering (H. Dosch and J. Peisl, Phys. Rev. Lett., 1986, 56, 1385-1388).
We present diffuse neutron scattering measurements on single crystals containing 2.5 at.% deuterium. Time of flight experiments using polarization analysis showed both elastic and inelastic scattering to be present. The latter was removed by using 4.3 Å neutrons with a beryllium filter behind the sample. Scattering from the deuterium-free crystals has been subtracted. The cross-sections have been compared with a Kanzaki force model of the displacement field.