conference abstracts

o.m10.p3 **Diffuse Scattering Associated with the Relaxation State in the $A_{II}B_V$ Compounds.** J.Sass, K. Mazur, *Institute of Electronic Materials Technology, ul. Wólczynska 133, Pl-01-919, Warsaw, Poland.*

The $In_{0.47}Ga_{0.53}As/InP$ epitaxial layers in the thickness range above the critical thickness were studied with triple crystal diffractometer. The measurements included careful recording of x-ray diffraction profiles and mapping of the intensity distribution in the reciprocal space. A special attention was paid to the diffuse scattering measurements in the vicinity of RLP, which enabled the characterization of misfit dislocation evolution. The present measurements revealed an additional maximum of diffuse scattering in ω-scan. It was found that that the angular position of the diffuse intensity satellites was independent from the misfit dislocation density. In the early stages of strain relaxation $\rho d \ll 1$ (ρ-linear dislocation density, d-film thickness) any shift of the layer peak on the relaxation line was observed.

o.m10.p4 **Diffuse scattering of a diatomic molecular system: comparison between the liquid and the plastic solid phases of oxygen.** O.B.M. Hardouin Duparc, F. Dunstetter, O. Condat, C. Clément, *Laboratoire des Solides Irradiés, Zcole Polytechnique - CEA - CNRS, 91128 Palaiseau Cedex FRANCE.*
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Molecular dynamics makes it possible to separate the various contributions of the total scattering. In the general case, these contributions produce rather complicated profiles with many peaks. Most of them can be related to the various atom-atom pairs found in the system, but no single peak can be ascribed to a given contribution, which makes it very difficult to analyse and to compare with the experimental data.

The case of diatomic molecules is unique since the intra-molecular atom-atom distance (about 1.1 to 1.4 Å) is much shorter than all the inter-molecular atom-atom distances (> 3 Å), with the result to separate more clearly the peaks of the diffuse scattering due to inter-molecular pairs from the peaks arising from intra-molecular pairs.

In the solid case, the intra-molecular diffuse scattering peaks are rejected towards the high-q range of reciprocal space ($> 6 Å^{-1}$) and the inter-molecular diffuse peaks are mainly located in the shorter q-range, typically from 2 to $5 Å^{-1}$. Moreover, the disorder strongly damps the inter-molecular diffuse peaks and their contribution becomes rather small in the high q-space domain whereas the intra-molecular contribution, only affected in its profile, has its maximal intensity in this domain. The result is to separate the inter and intra-molecular contributions in two distinct parts of the reciprocal space: the low-q and high-q domains.

It is however important to notice that a low-q inter and intra-molecular contribution mixture also exists in the solid: it can be found in the Bragg peaks.

The liquid case is thus more complicated: the Bragg peaks of the solid phase disappear and the related intensity is now distributed between the inter and intra-molecular diffuse contributions in the low and high-q domains.

Thereby, the balance between intra-molecular and intermolecular contributions to the total scattering is shown to be different in the plastic solid phase and the liquid phase. More precisely, the nature of the first diffuse peak at $2 Å^{-1}$ is a mixture in the liquid phase, whereas it is quite purely inter-molecular in the solid (in this region, the intra-molecular contribution is in the Bragg peaks). The second diffuse peak at $4 Å^{-1}$, weaker and broader in the liquid phase, is related to inter-molecular contributions. The third diffuse peak at $6 Å^{-1}$ is mainly of intra-molecular origin in both phases, but an inter-molecular contribution still exists in the solid phases.

The results of the simulation is compared with experimental data. Various contributions, also related to their translational and/or orientational origin, are discussed.