COHERENT AND INCOHERENT X-RAY SCATTERING FROM PARTLY RELAXED SEMICONDUCTOR STRUCTURES POSSESSING DISLOCATIONS

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A method is proposed to determine the concentration and relaxation depth profiles in graded epitaxial films from x-ray reciprocal space maps (RSMs). Various approximations in the kinematical x-ray diffraction from epitaxial films with the misfit dislocation [1,2] density depth profile are further developed. We show that a symmetric and an asymmetric RSM, or two asymmetric RSMs, contain enough information to obtain the concentration, relaxation and lattice tilt depth profiles without any additional assumptions. The proposed approach is demonstrated on the simulation of RSMs from $In_{1-x}Ga_xAs$ /GaAs and $GaAs_{1-x}P_x$/GaAs epitaxial graded films. The symmetric and asymmetric reciprocal space maps were also simulated for the samples with the fully coherent layer, in the vicinity of the critical thickness of relaxation, and with the fully relaxed layer. The crystallographic layer miscuts, indium concentrations, the relaxation degrees and density of dislocations have been included in simulation algorithm.

Another set of simulation of the high-resolution X-ray diffraction has been performed for multilayered $Si_{1-x}Ge_x$ heterostructures grown on (001), (011) and (111) Si substrates [3]. Reciprocal space map simulations demonstrate the influence of the strain and Ge concentration depth profiles within each layer of the heterostructures. The ratio of misfit to threading dislocation densities is shown to be distinguished for each individual layer based on the presence of diffuse X-ray scattering from the defects.

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