PS-13.03.02 ELECTRONIC STRUCTURE OF SUBSTITUTIONAL DEFECT PAIRS IN THE II –VI SEMICONDUCTORS

Xiaojiang Wu, Zihua Tian, and Qing Zhou
Department of Physics, Yunnan University, Kunming 650091, People's Republic of China

ABSTRACT

Deep traps lying within the fundamental band gaps greatly influence the electrical and optical properties of semiconductors. Understanding traps has been recognized as a very important problem in semiconductor physics for a long time. In recent years, the tight–binding Koster–Slater Green's function technique has been proven very successful in studying various properties of defects. Not only point defects, but also paired defects and extended defects have been studies widely. In this paper, employing the on–site tight–binding Koster–Slater Green's function method, the A_1symmetric deep levels and wavefunctions of a few series of paired substitutional sp^3–bonded defects in the II –VI wurtzite semiconductors CdS, CdSe, and ZnSe are presented. The chemical trends in the deep levels and wavefunctions, as the spectator defect varies, are predicted. A simple molecular model is used to describe the basic physics of the defect–paired problem.

ACKNOWLEDGEMENT

The project was supported by the Education Commission of Yunnan Province, China.

PS-13.03.03 COPPER ION POINT DEFECTS IN POTASSIUM SODIUM STRONTIUM BARIUM NIOBATE CRYSTALS. By Jiang Quanzhong*, Sun Daliang and Chen Huanchu, Institute of Crystal Materials, Shandong University, JINAN 250100, PR. China.

We have used a number of experimental techniques to identify the role that copper ion point defects play in potassium strontium barium niobate (KNSBN). Although they form deep energy levels and reduce the electron mobility, these defects obviously improve the photorefractive time response performance of KNSBN crystals. We attribute this phenomenon to the fact that many more photoelectrons induced by the LASER beams have taken part in the photorefractive process which results in the obtention of an equilibrium in a shorter time than in a copper ion-free KNSBN. Furthermore, these defects can also act as electron acceptors to improve the effective photorefractive charge concentration. In this way, the photorefractive properties of KNSBN are modified.

PS-13.03.04 **THE CRYSTALLOGRAPHY AND OBSERVATION OF ANTI-PHASE DOMAINBOUNDARY TUBES IN SUPERLATTICES. By N.Jiang*§† and Y.Q.Sun ‡, § Beijing Laboratory of Electron Microscopy, Chinese Academy of Sciences, Beijing 100080, China. † Dalian university of science and Technology, Dalian, China. ‡ Department of Materials, University of Oxford, Oxford OX1 3PH, England.**

Anti-phase domain boundary (APB) tubes are line defects which are unique to ordered superlattices and are not present in disordered systems. This article reports the latest progress on the crystallography, the dislocation mechanisms and the TEM observations of APB tubes in a number of superlattice structures, with an emphasis on the $L1_2$ structure to which Ni_3Al and Ni_3Ga belong. Existing dislocation mechanisms for the formatio ,n of APB tubes have been critically re-examined by taking into account the elastic interaction, as well as the crystallography of dislocation reactions and intersections. Single crystalline samples have been deformed under controlled conditions and the structure of APB tubes and their relation to the associated dislocations have been observed in TEM. Contrast analysis has shown that in addition to the APB displacement, an APB tube also possesses a long-range distortion field, on the basis of which experimental observations have been characterised. In Ni_3Ga, APB tubes have been found in samples with and without the presence of a secondary slip system. In the regime of single slip, APB tubes have been found to end at edge dipoles and this has been explained in terms of the incomplete annihilation of screw superdislocations involving cross-slip. When a secondary slip system is present, many APB tubes end at short dipoles of the intersecting dislocation system. The later feature is thought to originate from a modified Vidoz-Brown mechanism. The results are related to the plastic properties of the materials investigated, in particular the phenomenon of the unusual yield stress anomaly which has been found in several superlattice structures.

PS-13.03.05 AMPLITUDE DEPENDENT INTERNAL FRICTION OF SPHALERITE TYPE SEMICONDUCTORS. By D. Klimm*, B. Tippelt and P. Paufler, Institut für Kristallographie, Mineralogie und Materialwissenschaft, Universität Leipzig, Germany.

By treatment of sphalerite type compounds with ultrasound we were able to reach plastic deformation by motion and multiplication of dislocations. Ultrasonic treatment of GaP and GaAs was performed by cementing the samples to quartz crystals and applying driving voltages up to 80 V to the quartz, yielding amplitudes of vibration ε in the samples up to $7 \cdot 10^{-4}$ at frequencies of about 100 kHz. If ε is sufficiently high, amplitude dependent internal friction due to dislocations can be observed by measuring the current flowing through the quartz. The amplitude dependence measured is not always in agreement with GRANATO-LÜCKE theory (Granato, A., Lücke, K., J. Appl. Phys., 1956, 27, 583-589 + 789-805), but can be explained with a slightly modified model.

Plastic deformation of predeformed GaAs:Zn samples by ultrasound could be reached at stresses which are in good agreement with uniaxial compression experiments (Boivin, P., Rabier, J., Garem, H., Phil. Mag. A, 1990, 61, 619-672). Stress where dislocation multiplication by ultrasound begins can be determined by a sudden change of internal friction. TEM investigation after predeformation of GaAs:Zn by uniaxial compression (ε_{pl}=1..5%) at 820 K and after subsequent ultrasonic treatment (σ=25..56 MPa, T=400..600 K) shows, that deformation by ultrasound begins at that stress, where sudden change of internal friction takes place. The rearrangement of dislocations, however, begins at lower stresses than that needed to reach multiplication.

