PREFACE

The behavior of n-type dopants in III-V compounds has been revealed as a very complex one. In 1968 Craford and coworkers described the problems encountered when studying the transport properties of GaAsP doped with sulfur. Basically, deep states, related to the donors, and thought to be energy levels associated with the higher conduction band minima, were detected. A marked decrease of the free electrons available as temperature lowered, and a persistent photoconductivity effect (PPC) at low temperatures, were observed. Since then, during the last 25 years, the behavior of donors in III-V alloys has been the subject of a very extensive research effort. From the interest in GaAsP alloys, the research emphasis switched to AlGaAs compounds, motivated by the industrial importance of AlGaAs/GaAs heterojunction (HJ) based devices. For Al mole fractions in the 20 to 40% range, where the HJ properties are optimized, it was found that deep donors limit the achievable n-type conductivity as compared to the GaAs case, and hysteresis and low frequency instabilities were produced as temperature was cycled. In their pioneering work, Lang and coworkers described such deep levels as complexes formed by donors (*D*) and an unknown defect (*X*); since then, these defects are known as *DX* centers. It was also ascertained that DX centers were detected in those high band gap III-V alloys that evolve with composition from direct to indirect gap.

As seeing it now, "the DX center problem", the behavior of donors in III-V alloys, has shown to be unexpectedly difficult to understand. It is well established today that the DX centers are generated by the isolated donor atoms themselves and that substitutional donors not only create shallow effective mass states. However, to determine the microscopic nature of the DX center is still a challenging problem. Very attractive models were put forward at the end of the eighties, explaining most of the experimental macroscopic properties, and introducing the idea that the DX center is negatively charged when in its ground state. A key point is that in this picture, the DX center is a negative-U center (negative effective Hubbard correlation energy). The significant differences for the various chemical donor species were also qualitatively explained by these models.

Once the idea appeared that the DX centers are negative-U defects, most of the experimental activity in the scientific community was directed to prove, or to discard, such a model. The subject of determining the charge state of a DX center in its ground state (negative- vs. positive-U), and the specific path (intermediate states) that the electrons follow from the conduction band to the deep traps (capture process), or viceversa (emission process), either under thermal or optical excitation, have been under intensive research during the last five years. Structure sensitive studies by magnetic resonance, extended X-ray analysis fine structure (EXAFS), and Mössbauer effect experiments were performed. Several other techniques (magnetotransport, deep level transient spectroscopy) were focused on problems of local environment and on probing the local DX potential.

After being part of the ESPRIT-BASIC consortium on DX centers, the authors have now undertaken the effort of presenting their very recent results and views after such research period. A series of comprehensive chapters, with a detailed effort of cross-analyzing the information obtained from the various experimental techniques, and containing a critical discussion of those results under the light of the theoretical models that are available, have been prepared. A significant amount of new results, not previously published, are also presented.

In the ESPRIT Basic Action 3168, together with getting basic knowledge, a very significant activity was dedicated to explore techniques to minimize the deleterious DX center effects. These efforts comprised ways of doping, of the selection of the optimum donor species, of studying new donors, of codoping, and of the use of alternative alloys to AlGaAs. These investigations also aimed to analyze and to understand in depth most of the suggestions and empirical results that were originated outside the consortium with the same objectives.

The present publication on DX centers is focused on the physics of DX centers studied in AlGaAs alloys. For these alloys a significant amount of information was available, and their technology was mature enough to insure that the DX centers were not masked by other defects. However, other alloys, like GaAsP, InAlGaAs, AlInAs and InGaP compounds, have partially been studied. Ideas and models extracted from the AlGaAs experience were compared to these results.

The main questions regarding the DX centers were categorized into three sections: *microscopic structure models* of the DX centers (atomic and electronic structure, the amount and nature of lattice distortion upon electron capture, the charge state of the DX center ground state); *fundamental properties* (thermal activation energy, capture barrier for electrons and holes, effects in magnetotransport, electron emission and capture kinetics, optical properties); and *minimization of DX effects* in III-V devices (optimum doping procedure, selection of donor species, alloy compositions and device structures that avoid/minimize DX deleterious effects). These topics are presented in six chapters of this book. Special chapters dedicated to other III-V alloys, and to critically discuss the experimental results versus leading theoretical models, have also been included.

This book is addressed to the community interested in the physics and engineering of semiconductors, including senior undergraduate and graduate students involved in III-V semiconductor materials and device research. The DX center is an excellent **case-study** of the behavior of donors in semiconductors. It has shown the practical importance of non-effective-mass donor states, and there are indications that a similar "defect generation" by dopants may be present in other semiconductor materials. The DX center problem has stimulated research and new ideas in various areas of semiconductor physics and technology: from calculations of deep level defects and the idea of spatial correlation of charged centers to the development of new HJ transistors. Because of the deleterious effects of DX centers in electronic and optoelectronic devices, this book will also be useful to engineers and scientists working on III-V technology in the industry.

The present publication follows the book edited by J. C. Bourgoin on "*The Physics of DX centers in GaAs*" (TransTech Publications, 1990), which represents the discussions on the topic up to the year 1989.

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