

Extended Defects in Germanium

Fundamental and Technological Aspects

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Preface

Extended defects in semiconductors are usually considered detrimental. In the early days of electronic devices, only polycrystalline material was available. In fact, germanium was the first material that could be grown dislocation free, the reason being its relatively low melting point. With the improvement of crystal growth, dislocation-free wafers became available and are nowadays the standard in the case of 200 and 300 mm diameter silicon substrates. In the future, there may even be a switch over to a 450 mm wafer size. In the case of Ge it is already feasible to grow 300 mm dislocation-free wafers. On the other hand, low-cost, solar-grade silicon material is characterized by the presence of a large density of extended defects: grain boundaries, twins, dislocations and stacking faults, which determine to a large extent its electrical performance and solar energy conversion efficiency. Other applications, like detectors for nuclear radiation spectroscopy, require a density of dislocations in the range of a few hundreds to thousands for a successful, high-resolution operation. It implies that depending on the application, extended defects may be present and, therefore, their electrical and mechanical effects should be studied and well-characterized. Giving the current interest in renewable energy, and in particular, solar energy, it comes as no surprise that the study of extended defects in semiconductors is experiencing a second youth, with a great deal of research activities going on world-wide, involving a growing number of young scientists.

At the moment, the main application of Ge wafers is space solar cells, requiring high-quality defect-free material. Ge can be a potential block-buster, as channel material for sub-22 nm CMOS. However, transistors will be made only on thin Ge layers fabricated on a silicon handle or carrier wafer. Whatever the fabrication technique of choice, i.e., epitaxial deposition, Ge condensation or smart-cut GeOI, extended defects may readily be formed, so that the understanding of the formation and the control of extended defects is of crucial importance in state-of-the-art Ge materials. The main reason for the formation of misfit and threading dislocations is the lattice mismatch between the substrate - usually silicon - and the epitaxial layer, which amounts to about

4.1% at room temperature for pure Ge. It implies that below a certain critical thickness, which is about 1 nm for Ge, the layer can be deposited pseudomorphically, i.e., defect free, while above this thickness, plastic relaxation at the epitaxial interface readily occurs. Depending on the growth conditions, misfit dislocations are formed with threading arms reaching through the layer to the surface. It is in the first instance that these threadings can be harmful for device operation and should be controlled to acceptable levels, either during growth or by a post-deposition annealing treatment.

On the other hand, extended defects may be created also during device processing, as it is known that certain steps like ion implantation, dry etching or device isolation create damage and/or stress which eventually, upon annealing, develop into extended defects. Also thermal stresses during processing may relax into dislocations or related extended defects. Whatever the application or device structure, p-n junctions are generally an inherent part of it and the fabrication method of choice in industry is by ion implantation, as it allows a precise control of the junction depth and sheet resistance. The penalty paid is the formation of point and extended defects, which are the result of the clustering of the displaced lattice atoms and the associated vacancies. This clustering occurs during the post-implantation annealing, necessary to activate the dopants.

In view of these issues, defect engineering has become a mature and exciting field of expertise in the silicon world but lacks thousands of man-years of research in the case of Ge processing. The understanding of processes like ion implantation-damage annealing or solid-phase epitaxial regrowth, point-defect engineering for dopant diffusion control, etc. are far less well-developed in the case of Ge and, therefore, require renewed interest. The concept of gettering, where beneficial use is made of extended defects to remove detrimental metallic contaminants from the active device regions, and playing a crucial role in yield engineering in the IC industry, hardly exists for germanium. It is the aim of this book to fill this gap and form a bridge between the fundamental material studies carried out mainly in the fifties and sixties and today's practice and research interests. Defect formation in state-of-the-art processing modules intended for sub 32 nm technology nodes will be used to illustrate the theoretical and physical defect studies.

The aim is to give an overview of the physics of extended defects in germanium, i.e., dislocations (line defects), grain boundaries, stacking faults, twins and $\{311\}$ defects (two-dimensional defects) and precipitates, bubbles, etc. The first chapter will be more fundamental, describing the crystallographic structure and mechanical properties of dislocations, which have been established in the fifties and sixties, based on defect etching and optical or electron microscopy. Currently, focus is on *in situ* studies of dislocation properties in a transmission electron microscope. It will be pointed out that dislocations are essential for the plastic deformation of germanium. Methods will be described to analyse and image dislocations and to evaluate their structure. Another field of interest is the measurement of strain distribution with nanometer

scale resolution. Indentation studies at room temperature are useful for the understanding of high pressure phase transformations in Ge and for revealing the hardness properties of Ge and related alloys. Dislocations can also impact on the diffusion of impurities, as will be outlined in the last paragraph.

The second chapter deals with the electrical and optical properties of dislocations, which are crucial for device operation. An overview of the different models, describing the electron states, will be given, starting from the dangling bond model of Shockley and Read. While over the years, large progress has been made, a full understanding is still lacking due to the complexity of the problem. Besides the presence of dangling bonds in the core of the dislocation, which may reconstruct, the states associated with the strain field may split from the band edges. Moreover, impurities tend to aggregate in the strain field of a dislocation, giving rise to greater recombination activity. The combination of optical and electrical spectroscopy has led to the concept where the dislocation states form one-dimensional bands in the band gap of germanium (or silicon) instead of a single level, which depends on the line charge captured in it. Chapter 3 describes the mechanical and electrical properties of grain boundaries in Ge.

Chapters 4 and 5 deal more with today's problems, namely, with the formation of extended defects during the preparation of modern Ge substrates, including epitaxial deposition on Si, condensation of SiGe-on-Insulator and smart-cut or bonded material and the issue of extended defect formation during modern processing, for example, by ion implantation or laser annealing.

In brief, the book should provide a fundamental understanding of the extended-defect formation during Ge materials and device processing, providing ways to distinguish harmful from less detrimental defects and point out ways for defect engineering and control.

Key features:

- Intended for a wide audience including students, scientists and process engineers employed in material manufacturing, semiconductor research centres and universities
- State-of-the-art information available for the first time as an all-in-source
- Extensive reference list making it an indispensable reference book
- Complementary to the first book on Ge Materials and Devices, edited in 2007 by the same authors.

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