Defects and Diffusion in Silicon Technology

Tony E. Haynes

The silicon at the heart of high-performance integrated circuits (ICs) is the most precisely engineered material in mass production today. Crystalline silicon, purified to the level required for manufacturing modern, high-performance microelectronics, is arguably the most perfect material known. It is produced in large quantities and very economically. Continuing progress in basic silicon materials science has been central to this achievement. At the same time, access to such perfect material and detailed knowledge of silicon's properties have provided the experimentalist with excellent opportunities to devise rather elegant experiments in which the parameters can be controlled very precisely. Silicon has similarly provided condensed-matter theorists with a nearly ideal testbed for new theoretical approaches. This issue of the *MRS Bulletin* is dedicated to the materials physics that has both enabled the development of such highly perfect material and benefited from its availability.

The stringent constraints placed on the properties of the silicon used in microelectronics pose a number of challenging problems for the materials scientist. Many of these demands come from the push for ever-increasing performance that drives the IC market. For instance, operation at higher frequencies with lower power consumption and in smaller packages constantly challenges our ability to control the placement of dopant atoms that determine the operational characteristics of individual transistors. Other considerations are related to more practical matters of economy and reliability that drive us toward improved strategies for reducing the number of manufacturing steps and increasing the manufacturing yield, i.e., fraction of completed devices that meet operating specifications. Solutions must also be found for controlling grown-in crystalline defects as well as defects and contaminants that are introduced into the silicon during manufacturing. The contributors to this issue of the *Bulletin* have provided a survey of the current status of some of the most interesting materials science problems that lie below the silicon surface.

The first article, by Paul Packan, provides an appreciation for the magnitude of the research challenges in today's silicon materials science by describing the critical link between the materials research needs and the limitations on continuing improvements in device performance. Calculations of the electrical properties of model transistors dramatically demonstrate how performance is limited by dimensional scalability. Extrapolation of current scaling trends shows that the continued success of scaling will depend very soon on the elimination of nonequilibrium dopant diffusion and electrical activation of supersaturated dopant concentrations.

These considerations lead naturally into a discussion of the properties of point defects in silicon that control diffusion and impurity clustering. Therefore, Hartmut Bracht's article provides an overview of our current state of knowledge of the fundamental properties of the intrinsic point defects (vacancies and interstitials) and of the mechanisms of self- and impurity-diffusion in silicon. This article provides the foundation for understanding the topics discussed in all the remaining articles.

Of course, it all begins with the starting silicon wafer. Silicon crystals are grown by cooling from a liquid melt. Relatively large concentrations of intrinsic defects and impurities are soluble in the solid at the melting temperature, but the solubilities quickly decrease during cooling. The temperature gradients that are encountered lead to gradients in the concentrations of the defects as well as some important impurities, chiefly oxygen, that must be carefully controlled in order for the silicon wafer to be useful. Therefore, many of the point-defect concepts used in dopant engineering are also important in wafer engineering. This point is made quite clearly in the article by Robert Falster and Vladimir Voronkov, who explain how fundamental knowledge of point-defect properties can be used to produce “perfect” silicon.

Unfortunately, even “perfect” silicon cannot remain so, chiefly because the manufacturing environment in which it is processed is replete with deleterious contaminants. Extreme efforts are taken to minimize the amount of potential contamination to which a silicon wafer is exposed. Nevertheless, there is so much investment at stake by the time a wafer has been through, say, 80 process steps, and is still not finished, that special methods are used to effectively immunize the active volume of the silicon against contamination that it may acquire along the way. The article by Andre Istratov, Henry Hieslmair, and Eicke Weber describes the physical and chemical processes involving control of point-defect and impurity fluxes and reactions that underlie the half-dozen or so gettering schemes in use today to provide this immunity.

The progress of device scaling is seriously threatened by the highly nonequilibrium nature of some of the process steps employed in IC manufacturing. As Nick Cowern and Conor Rafferty point out in their article, point-defect supersaturations of hundred- or even thousand-fold are created following ion implantation, which is used to introduce the dopants into silicon. Other common processes such as oxidation or silicide reactions also perturb the equilibrium to a lesser extent. Such supersaturations dramatically alter the diffusion of the dopants and can reduce their electrical activity, with severe consequences for device operation. On the other hand, while these large perturbations are a nuisance in silicon processing, they simultaneously provide opportunities for researchers attempting to understand the fundamentals of point-defect dynamics because the same processes can be used to produce intentional supersaturations to alter the point-defect concentrations in controlled experiments. Cowern and Rafferty summarize the current standing of the tremendous amount of effort that has been directed over the last 10–15 years to both understand and control these nonequilibrium phenomena in detail.

The true test of our understanding in any materials science subfield is whether or not that understanding is predictive and accurate. The final article in this issue, by Mark Law, George Gilmer, and Martin Jaraíz Maldonado, discusses the state-of-the-art in the development of predictive computational tools to describe point-defect related phenomena in silicon. The complexity of the problem is immense– this is illustrated by the significance of nonequilibrium behavior and the fact that tens or hundreds of different process steps may interact. This complexity dictates that pieces of the problem must be tackled using different computational approaches, and this article describes the interrelationships among different components of what is developing as a coordinated, hierarchical computational strategy to predict point-defect interactions in silicon processing.

In the present case, the computational test of our understanding is not merely an academic exercise. The economics of silicon processing will soon require that truly predictive capability must become available for the industry to advance. It has become prohibitively expensive to test a new process by running real wafers through a multibillion-dollar fab. It is far preferable to run the test on a workstation, but only if the predictions are reliable. The success of predictive calculations, which must be founded on the basis of solid, detailed understanding of the physical processes as outlined in the other articles in this *Bulletin*, may well determine whether the challenging barriers to scaling outlined by Packan can be overcome.

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