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The real situation is more complicated because other impurity atoms will be present, particularly oxygen which is bonded or anchored to two silicon neighbors but is located in the spaces or interstices between the silicon atoms. The oxygen strains the crystal in the opposite sense from carbon, and the two types of impurity prefer to occupy adjacent sites as this leads to an overall reduction in the strain. To form such pairs the carbon impurity would have to jump from one lattice site to the next, but this is not easily achieved because the atoms of the crystal are in the way and an exchange process must occur. On the other hand, for atoms in interstitial sites where the bonding is weak, migration through the crystal can proceed much more readily.

When silicon crystals are bombarded with nuclear particles, collisions occur and some atoms are knocked off their lattice sites into the interstices. Carbon impurity atoms are very readily transferred during this process and can then migrate even at room temperature. They are then trapped at other imperfections in the crystal including undisplaced carbon and oxygen atoms to form a whole series of complicated clusters of impurities. It is crucially important to understand the structure and nature of such defects because they can have detrimental effects on the properties of silicon used to make (a) integrated electronic circuits or (b) devices for power circuits.

In this paper, we review the current state of knowledge of these effects in silicon immediately after its growth, and following various processing, including high-energy bombardment and heat treatments at elevated temperatures which can also lead to displacement of carbon atoms from lattice sites. The processes are monitored mainly by measurements of transparency of the crystals with optical equipment operating in the infrared spectral region. This diagnostic method can be understood by comparison with other materials that are transparent to visible light. The presence of defects or impurities in such a material, including glass, removes light at certain wavelengths and the material acquires a characteristic color. The view of silicon in the infrared is similarly "colored" by the defects involving carbon and the color changes produced by processing tell us which types of defect have been produced or destroyed. Colors characteristic of several defects have been identified but considerbly more research effort will be needed before a full understanding can emerge.

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Special-Purpose Computer for Molecular Dynamics

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Physical systems have traditionally been analyzed by searching for functional relationships between various measurable parts of the system such as the density, temperature, particle forces, etc. These functional relationships are represented by complex mathematical functions which are then analyzed by classical methods for the solution of the integro-differential equations. Analytic solutions thus obtained can then be evaluated on a computer to obtain numerical results for further study. This method is severely limited when applied to many interacting particles because of the huge number of equations which would be required and because the solutions, when obtainable, are the sum of a large number of functions.

With the advent of high-speed digital computers it is feasible to approach the understanding of physical systems by a direct calculation of the behavior of each individual element of the system, from which global parameters can be derived. This is possible because the computer has the unique ability to keep track of a very large amount of information at the same time and also because it is much faster at simple calculations than the scientist. A direct calculation of the behavior of each atom or particle in a material based on its motion over a very short period of time can be easily written as a large number of simple equations. This approach to materials properties has been dubbed, "molecular dynamics" and is one example of the general approach to solving problems by direct simulation of the behavior of each element of a system.

Such an approach is not a panacea, however, when the amount of brute-force calculation required to simulate even simple systems is considered. For example, it is easy to show that a computer which is capable of computing the interaction of any pair of particles in a system as small as a grain of table salt in one-millionth of a second (a microsecond) would require 10^{44} years of calculation to simulate the salt crystal for one second of real time, since each atom in the grain interacts with all other atoms.

Obviously, compromises must be made to achieve a reasonable computation time. Study has shown that a good model of a crystal can be made with about 1000 atoms. In addition, it is sufficient to study the crystal over shorter periods, say 0.001 second. With these new numbers a reasonable computation can be carried out in about one year if we can afford the full-time cost of a super-minicomputer for that period.

Since a computer must be virtually dedicated to a single problem for simulations of this size (and hopefully much larger) it is logical to build a special-purpose computer which is better at simulation than a general-purpose computer. Such an approach is made feasible with the availability of inexpensive, monolithic computing elements which each have a computation speed comparable to the arithmetic component of a superminicomputer.

The calculations that must be carried out in molecular dynamics between each pair of particles is relatively simple, so it is practical to provide a large number of these computing elements to achieve a further increase in computing speed proportional to the number of arithmetic processor elements used. In this way, computations for different particles are carried out simultaneously by different computer processors. Since the computations carried out on different particles are virtually the same in a molecular dynamics calculation, such a problem is ideal for the application of multiple processors.

The use of multiple processors in this way is called parallel processing, and is being widely applied in the computer industry today. There are many problems in achieving a practical parallel processor system related to the transfer of information between processing elements. However, there is a great cost advantage in building a parallel processor system when the class of problem that must be computed

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is well defined, because it is not necessary to duplicate an entire computer system many times in order to achieve parallelism.

We have designed and constructed an experimental parallel processor at the State University of New York at Stony Brook which can achieve a large degree of parallelism using a modular format for the arithmetic processors and their associated memories. Necessary communication between the several processors is made over multiple, very high-speed computer links which run at full speed simultaneously. The couple parallel computing elements are run under synchronous control of a single host computer which sends the computational routines to the processors before a computing session begins and which also provides data for the computation, such as particle forces and initial positions. As each task is completed, such as updating the positions and velocities of about 20 particles for each processor, the host control system redirects each processor to a new task or a new group of particles. This process takes about one microsecond. In most cases, all processors are redirected within the same microsecond.

Our test results show that computational capabilities can be achieved in a relatively inexpensive machine which greatly exceed the speed of super-minicomputers which cost a hundred times as much. For example, a 16-processor parallel computing engine with a modest host computer will cost about $55,000 and has the computational speed of 80 million instructions per second. In addition, the modular nature of the design makes it possible to connect as many 16-processor modules together as the problem warrants with only a slight change in the software. When these features are combined with the full-time availability of this computer to the scientist because of its low cost it can be seen that a completely new range of simulation becomes practically possible.

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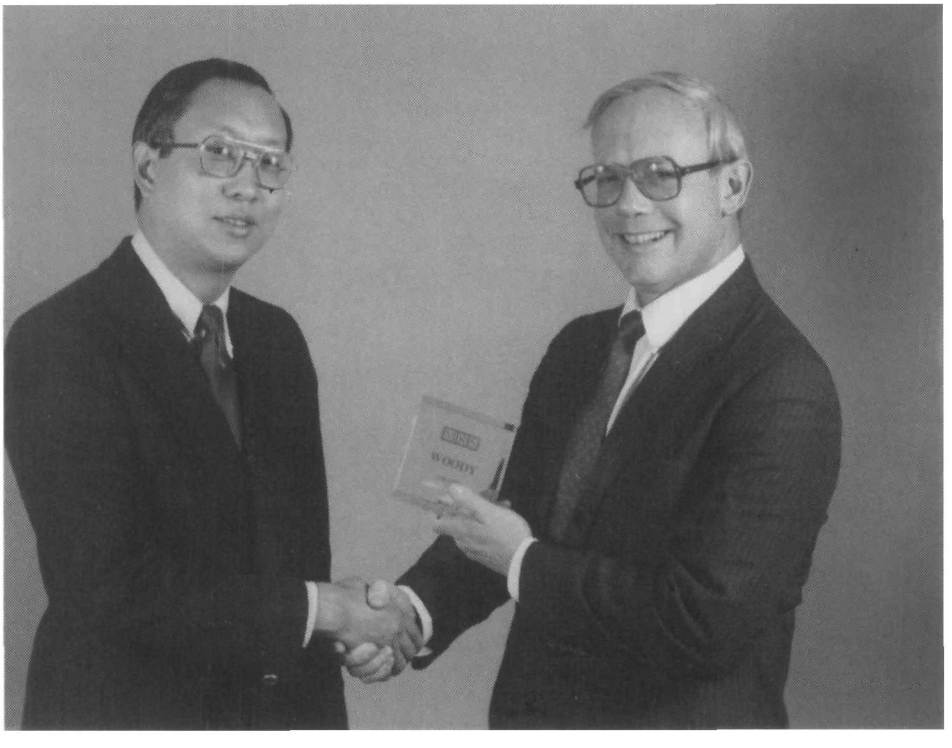
Leamy Receives 1985 Woody Award



Harry Leamy (right) receives 1985 Woody Award from Bob Chang.

Awards Committee Chair Woody White announced to the Council during the Fall Meeting in Boston that Harry J. Leamy, AT&T Bell Laboratories, was the 1985 recipient of the MRS Woody Award. The award is bestowed annually to a member of the Society for outstanding organizational talents, energy, and service to the Society.

R. P. H. Chang presented the award to Leamy in early January at Bell Labs. Speaking on behalf of the Society, Chang said, "The Council, Officers and membership have benefited a thousand-fold from your contributions. The award is but a small token of their appreciation for the critical role you played in starting the **MRS BULLETIN** and the conference proceedings series, launching the effort which resulted in the MRS Headquarters, starting the Laser Annealing Symposium, serving as meeting chairman for the highly successful 1981 Boston Meeting, and all the many contributions made as President in 1983, Vice President in 1982, and Chairman of the Publications, Long Range Planning, Awards, and Nominating Committees at various times during the last five years."

"Above all," Chang said, "the award is given for your incredible ability to attract other dedicated individuals to become actively involved in the Materials Research Society."

Ironically, it was Leamy who instituted the Woody Award over a year ago to recognize individuals whose dedication to materials research is exemplified by outstanding service to the Society. The award is named after its first recipient Woody White, 1984 MRS President.

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