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LEHIGH UNIV BETHLEHEM PA DEPT OF PHYSICS  
RADIATION DAMAGE PROCESSES IN SILICON (U)  
1981 G D WATKINS

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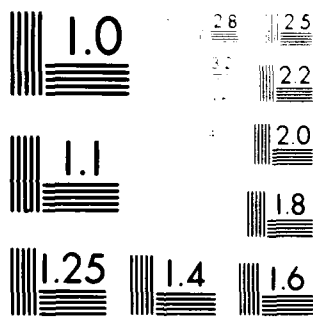


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TITLE: ⑥ Radiation Damage Processes in Silicon

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**OBJECTIVE:** The basic objective is to understand the electronic properties of simple point lattice defects in the silicon lattice, the mechanisms by which they are formed, and the processes by which they can migrate through the lattice and react with other defects to form complexes.

**APPROACH:** The primary technique for producing defects is high energy electron irradiation (1-3 MeV). These irradiations are performed *in situ* at cryogenic temperatures to freeze in the primary defects for study and to separate the production mechanisms from the complex defect reactions when migration and annealing take place. Electron paramagnetic resonance (EPR), optical spectroscopy, and transient capacitance spectroscopy (DLTS) are the principal experimental techniques used in the study. The effects of charge state and electronic excitation on the stability, mobility, and reaction kinetics of various defects are studied. Theoretical calculations of the electronic structure of these deep level point defects form an integral part of the study.

**PROGRESS:** (During the period 10/1/80-9/1/81): Combined DLTS and EPR studies have located the positions of the donor and acceptor levels of interstitial boron and confirmed unambiguously that the levels are inverted from normal ordering. Interstitial boron therefore becomes the first and only identified defect with negative-U properties in any solid. Similar studies are currently underway to probe our suggestion that the lattice vacancy also has this property.

Careful study of the recombination-enhanced migration of the lattice vacancy has provided direct evidence that the motion is taking place when the vacancy is in a positively charged state. This suggests that the driving force is the large tetragonal Jahn-Teller distortion known to occur from EPR studies for the  $V^+$  and  $V^0$  states. This raises the interesting theoretical question as to how this energy is so efficiently funneled into the trigonal diffusive mode.

A systematic DLTS study of the emergence of interstitial carbon after low temperature irradiation and anneal of n-type silicon has been performed. Complex charge state and injection level dependences are observed which we conclude are reflecting the properties of interstitial silicon as it is released and migrates to be trapped by the carbon in competition with other traps. This is part of a study to unravel the properties of interstitial silicon, so far almost a complete mystery.

Scattered wave X- $\alpha$  calculations for clusters simulating interstitial transition element impurities in silicon are in progress. Inclusion of many-electron effects provide remarkable agreement of level positions with experiment. MNDO calculations are underway on clusters to probe the physical origin for off-center displacements of substitutional first row element impurities (O,N,C) in silicon.

**PUBLICATIONS:**

1. G. D. Watkins, A. P. Chatterjee, and R. D. Harris, "Negative-U for Point Defects in Silicon," in Defects and Radiation Effects in Semiconductors 1980, (Inst. Phys. Conf. Ser. No. 59, 1981) p. 199.
2. G. D. Watkins, "Summary of the 1980 Conference," in Defects and Radiation Effects in Semiconductors 1980 (Inst. Phys. Conf. Ser. No. 59, 1981) p. 139.
3. G. G. DeLeo, G. D. Watkins, and W. B. Fowler, "Theory of Interstitial Transition-metal Impurities in Silicon," Phys. Rev. B23, 1851 (1981).
4. G. D. Watkins, "Negative-U Properties for Point Defects in Silicon," in Defects in Semiconductors, edited by J. Narayan and T. Y. Tan (North Holland, New York, 1981), p. 21.

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PERSONNEL: (10/1/80-9/1/81)

Faculty: Professor George Watkins 1 month summer  
 Professor W. Beall Fowler 3-1/2 weeks summer  
 Post Doc: Gary DeLeo 50% time  
 12 months

Research Sci/  
 Engineer: None

| Graduate Student: | Name          | Academic Year          | Summer        |
|-------------------|---------------|------------------------|---------------|
|                   | A. Chatterjee | 50% @ 462/mo + tuition | 100% @ 740/mo |
|                   | R. Harris     | 50% @ 462/mo + tuition | 100% @ 740/mo |
|                   | J. L. Newton  | 50% @ 462/mo + tuition | 100% @ 740/mo |
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PROPOSED RESEARCH:

The difficult task of determining the electrical level positions for the lattice vacancy will be begun. In addition to probing the possible negative-U ordering of the single and double donor levels, attempts will be made to locate the deep single and double acceptor levels. Wavelength dependent photocapacitance studies will be begun in conjunction with EPR studies under photoexcitation.

DLTS and EPR studies will be continued on processes directly or indirectly related to interstitial silicon. Damage processes in the temperature range  $\approx 100K$ , known to be different, may provide new insight into this question.

In the theoretical studies, the complex question of cluster termination and how best to simulate the rest of the semiconductor will be explored. The study of lattice relaxations, off-center distortions, etc., will be continued. Exploratory calculations to predict defect configurations and the role they play in negative-U ordering, recombination-enhanced migration, etc., will be begun.

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