RADIATION KINETICS IN ELECTRONIC MATERIALS

Semiannual Report

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The degradation of minority carrier lifetime in solar cells irradiated in a space environment is an important problem in aerospace technology. It is also an interesting physics and materials problem to account for the manner of degradation, recovery, and redegradation with the technological goal of optimizing solar cell performance.

The development of lithium-diffused solar cells, following the demonstration of Wysocki[1] and others that such cells may spontaneously recover, occupies a unique position in material technology--an example of full (or almost full) recovery in an irradiated, technologically-important material at room temperature. The mechanism by which lithium affects this recovery is still clothed in a good deal of doubt.[2,3,4] Some of the difficulty arises from the nearly inherent properties of silicon, for example the ability of small amounts of oxygen (and other impurities) to influence damage and recovery in a most significant manner. Studies in the near-liquid nitrogen range (i.e., well below room temperature) show the presence of a complicated set of defect centers, presently referred to as ITD and ITI (irradiation temperature dependent and irradiation temperature independent, respectively) defect centers.[5]

In order to approach the further development of solar cells, it is necessary to bring the observations regarding degradation, recovery, and redegradation into order by placing these observations into an analytical frame work. Inevitably this is approached by the structuring of models into which the important parameters are introduced. We are concerned with the formulation, structuring, and solution of such models.

The most extensive work of this nature has been performed by

Fang and colleagues but their formulations have either been highly mathematical in nature (making comparison with experiment almost impossible) or directed toward assumptions which are generally ad hoc in nature, such as a concentration-dependent energy at low defect concentrations.[7]

In our work we have sought kinetic models which would be based on assumptions which seemed more realistic to us and which would yield results which could be compared directly with experiment. It has not been our intention, however, to <u>over</u>-simplify the situation. In fact, we have been motivated by the possibility that models based purely on chemical rate equations, with no regard for spatial dependences, may be seriously flawed from the beginning. We are not the first to bring the possibility to light. Brucker, et al.[8] have already applied the simpler elements of a full diffusion theory formulation, due to Waite,[9] to the problem with some success. Since we have developed the problem beyond the work of Waite and developed the computer programs to test models based on this approach, we were (and are) prepared to evaluate the importance of diffusional aspects in solar cell damage and recovery.

Nevertheless, it is vital to begin such an approach with a model and models must be based on existing experimental observations. On examination of the data,[6,10,11,12] we have become conscious of the disparity in reported data, probably due to variations in sample fabrication methods and experimental techniques. In some cases there appears to be a clear contradiction between the work of different investigators--in particular in regard to the question of recovery time versus defect concentration.[6,10] Nevertheless we feel the following facts to be of importance.

1) For a large portion of the recovery from radiation damage it is

the short circuit current and not the concentration of defects which is reported to have a simple time dependence.[6] We will henceforth refer to this phase as phase A.

2) Phase A is characterized by a dose independent annealing time at room temperature (about 1×10^4 sec). The fraction of damage recovered in Phase A depends on the dose. The larger the initial damage the smaller the fraction annealing.

3) It appears that the initial phase is followed by a second for which the effective recovery time increases with increasing initial damage.[6] We will refer to this phase as phase B. The data regarding phase B is in conflict. Brucker[10] et al. found 1st order kinetics for this region which would predict a dose independent annealing time. However, their data is for low damage where the dose dependence is much less pronounced.

4) The "recovery times" associated with the two phases are strong functions of the exact composition of the cell.[10]

We have, as discussed in a previous report, analyzed the significance of the simple time dependence in an elementary kinetic model in hopes of reaching conclusions concerning the nature of the defect configurations. The result is a formal development which includes the conditions outlined above but, unfortunately, provides little information concerning the underlying mechanisms. We have, therefore, discontinued this approach. However, we have also previously concluded that a second process appears to be occurring at longer times. This may be consistent with the observations of Stannard of the Naval Research Laboratories who has pointed to the existence of a deep acceptor level, still unidentified.

It appears that our original goal--to follow the recovery in a photocell using a "full diffusional analysis"--is the most profitable procedure. This analysis is presently fully implemented for a parallel study in radiation damage in metals; our immediate task is to bring into the development a number of features which are needed for the solar cell problem.

Computer based reaction kinetics:

The program presently being used to study annealing in metals allows for a number of reactions. In this case, the following reactions, typically, may be included:

1. Interstitial-vacancy interaction
2. Interstitial-interstitial interaction
3. Interstitial-impurity interaction
4. Release of bound interstitials from near-impurity sites.
5. Interstitial-dislocation interaction
6. Formation of interstitial clusters of order three or greater.

Other related reactions could be inserted with no difficulty. These reactions are treated in a manner closely related to chemical rate rate theory but which accounts for transient features of diffusion theory as well. In addition, the treatment of non-homogeneous distributions of interstitial-vacancy separations is included as still another term in the coupled differential equations which characterize this problem.

A simplified flow diagram of the program is appended to this report. The significant features of this program for the study of recovery in metals are the inclusion of a relatively large number of competing reactions, the "proper" formulation based on diffusion theory (a feature necessary to accommodate non-uniform distributions), and the simplicity and completeness of the final computer output (tabular or graphical).

The extension of this program to semiconductors and, more particularly to solar cells, requires some modifications and additions. At the present, the main parameters which we intend to include in the program are the concentrations of lithium, oxygen, vacancies, and, perhaps, other radiation-produced electrical centers. Furthermore, the electronic state of each of these reactants must be treated separately: Li vs. Li^+, V vs. V^-, etc. plus the inclusion of hole and electron concentrations. Notice that these inclusions allow us to treat both damage processes and recovery processes since the most commonly accepted reactions are

$V + Li^+ + 2e^- \rightarrow (Li\text{-}V)^-$ during damage

$Li^+ + (Li\text{-}V)^- \rightarrow Li\text{-}V\text{-}Li$ as a recovery step

There is also some evidence that the reaction

$$V + Li^+ + e^- \rightarrow (Li\text{-}V)$$

plays an important role in damage processes. Which of these two reactions is appropriate presumably depends on the position of the Fermi level; this can also be included in the analysis.

The major problems which we foresee in pursuing this course arise from the following:

1. Non-uniform distribution of lithium, recombination centers, and electrical carriers in the junction region certainly play an important roll in establishing solar cell characteristics. Inclusion of these non-uniform distributions remains to be considered.

2. Closely related to the above point is the consideration of non-uniformities imposed by strain fields and local electrostatic fields.

3. In comparison with observations, it must be recognized that the parameters included into this program are most inadequately determined.

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