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FINAL TECHNICAL REPORT

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Dislocations in Solids

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Scientific

During the two year period of this contract, we have completed four of the projects which we were already working on at the start. These are listed below with a short description of each.

1. Theoretical studies of discrete dislocation models. During the early part of the contract period, Hobart and Celli completed a study of a one dimensional discrete dislocation, and its motion. This work was primarily Hobart's thesis, but Celli suggested an important method for reducing the equations. The object of this work was to study the dynamic aspects of the discreteness of dislocation cores. This is a very difficult problem, and our work was only partially successful in approaching the major goal. Hobart was able to develop techniques which worked only when the dislocation motion was not too fast. It may be of interest that Hobart has continued in this general area, and has since developed his technique in the direction of the motion of diffusing atoms. This extension of his earlier work looks very promising.

2. Theory of Climb. This work was carried out jointly between the principle investigator and Professor R. W. Balluffi of this department. The point of departure in this work was to treat the problem of the detailed kinetic nucleation of jogs and absorption of vacancies by a dislocation line. We developed a general framework and a mathematical description of the process which even included the fact that interstitials are a necessary part of the problem for

equilibrium to be possible. From the mathematical apparatus, it was possible to obtain rather simple equations for the rate of climb of a dislocation which included a number of parameters such as the pipe diffusion rate, jog formation energies, etc. The object of this work was to see if there were circumstances where one could hope experimentally to measure such parameters as the pipe diffusion rate and jog nucleation energies. Just recently, work by D. Thompson at Oak Ridge seems to point the way to just this possibility, though his work goes in a slightly different but related direction to what we had in mind.

3. Pipe Diffusion in LiF. Tucker and Laskar carried out an experimental program to measure the pipe diffusion of Na impurities along dislocations in LiF. By a series of different types of measurements, they were able to measure the diffusion rate and activation energy for the process. The theoretical implication of this work is that the dislocations in LiF must have either large densities of vacancies in the core, or that the core is actually hollow. The diffusion rate along these dislocations is surprisingly rapid.

4. Dislocation Mobility in Ge. Kabler measured the velocity of individual dislocations in Ge as a function of temperature and stress. A feature of this work was his ability to separate out the screw dislocations from the 60° by an indirect method based upon the geometry of the glide process and the difference in velocity between the two types. He was also able to show by etching in the slip plane of the

crystal that the dislocations move with long straight segments parallel to the (110) directions of the crystal. This demonstrates conclusively that the Peierls energy is the dominant factor in the velocity. We have developed a theory to account for the stress and temperature dependence of the dislocation velocity. The model involves the nucleation of kinks in the dislocation which cross the Peierls valleys and the interaction of these kinds with inhomogeneities along the dislocation which act as pinning points for the kinks. A feature of this theory is a detailed treatment of the statistical mechanics of the kink nucleation problem. We have developed an explicit formula for the kink nucleation rate including the normally vague frequency factor. Our theory should be generally valid in crystals where the Peierls energy is the dominant factor, and recent evidence that iron is such a case has made us interested in extending our work to that case.

In addition to these four major efforts which have been completed, we have been deeply involved in the problem of the influence of dislocations on the electronic energy states of the solid. At the present time, this is our major preoccupation. Celli, Gold and the principle investigator used the deformation potential in Ge to calculate the trapping level on the screw dislocations in that crystal. During the past summer, Usmani working with Celli and the principle investigator, extended this work to the 60° dislocations in calculations which included such subtleties as the anisotropic strain field around the 60° dislocations. All of this work yields trapping levels which are more shallow than those which have been experimentally observed. We have therefore adopted the view that in the case of the screw dislocations, where there are no dangling bonds, the self-consistency of the continuum approach suggests strongly that there should be a trapping level about where we have predicted it. However, in the 60° dislocations, the presence of dangling bonds impairs the validity of the work. The work shows, however, that the dangling bonds have a strong perturbing effect on the level. We are planning to make a major project to calculate these dangling bond effects. In addition to the theoretical work Ninomiya and Meyer have been setting up experimental apparatus to make measurements on the optical properties of pure screws in Si and Ge. Unfortunately, this work has not progressed far enough to have obtained results as yet, beyond the fact that we have been able to get crystals with nicely developed screw dislocation networks.

Financial

We have ended the contract period with an estimated $6,000 in unused funds. This surplus occurred even after a three month no cost extension of the contract. The primary reason for the large surplus has been the unavailability of personnel. For most of the period, the number of post-doctoral people has been up to planned strength, but the number of students on the payroll has been consistently lower. We have had some difficulty on this score, having lost three graduate students through attrition in their studies. This is a rather unusual loss ratio and could not have been predicted. In addition, during the past several months, the spending rate has been lower than planned because: (a) an expected post-doctoral man has been three months late in arrival due to health reasons; (b) travel costs to the international conference in Japan was paid by the NSF; and (c) an expected charge for a desk calculator was not necessary because one has been furnished by OSR.

Travel

During the contract period, various members of the group attended the Solid State meetings of the Phys. Soc., where various submitted papers were delivered concerning work then in progress. In addition, the principle investigator attended the conferences in Tokyo and Kyoto, Japan in the fall of 1962 on lattice defects, where the results of our work on germanium dislocation velocities and on pipe diffusion were presented.

Publications

Articles:

1. Energy-Band Structure of Solids from a Perturbation on the Empty Lattice, V. Celli and F. Bassani, J. Phys. and Chem. Sol., 20, 64, (1961). (This work, though published during the contract period, was performed for the most part during the previous year under a previous OSR contract.)

2. A Solution to the Frenkel-Kontorova Dislocation Model, R. Hobart and V. Celli, J. Appl. Phys., 33, 60, 1962. (This publication was the outcome of Hobart's thesis.)

3. Kinetic Theory of Dislocation Climb, I, General Models for Edge and Screw Dislocations, J. Appl. Phys., 33, 803, (1962).

4. Kinetic Theory of Dislocation Climb, II, Steady State Edge Dislocation Climb, R. W. Balluffi and R. Thomson, J. Appl. Phys., 33, 817, (1962).

5. Electronic States on Dislocations in Semiconductors, V. Celli, A. Gold, and R. Thomson, Phys. Rev. Lett., 8, 96, (1962).

6. Pipe Diffusion in LiF, R. Tucker, A. Laskar and R. Thomson to be published in J. Appl. Phys., (1963).

7. Pipe Diffusion in LiF, (shorter account than above, to be published as part of the International Conference on Lattice Defects, Japan, 1962, in Proc. Phys. Soc., Japan).

8. Dislocation Mobility in Ge, I, Experimental, M. Kabler, to be submitted for publication next month.

9. Dislo cation Mobility in Ge, II, Theory, V. Celli, M. Kabler, T. Ninomiya and R. Thomson, to be submitted with 8, above.

10. Mobility of Dislocations in Ge, V. Celli, M. Kabler, T. Ninomiya, and R. Thomson, to be published, as part of the proceedings of the International Symposium on Mechanical Properties, Japan, Proc. Phys. Soc. Japan, 1963. This is a shorter account of the work of items 8 and 9.