MIGRATION OF VACANCIES TO STRESS CENTERS

Thesis by

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ABSTRACT

The activation energy for motion of a vacancy in an edge dislocation width is considered by a modification of the method of Bartlett and Dienes. The results indicate an expected trend of motion toward the center of the width in the compressed half with a decreasing activation energy from edge to center. On the basis of the model used there is little tendency to form nonequilibrium vacancy doublets by this mechanism.

TABLE OF CONTENTS

I. INTRODUCTION

It has been suggested that the mechanism for the formation of fatigue "cracks" in the initial stage may be associated with the nonequilibrium production of vacancies through mechanical means. In this connection it may also be interesting to consider the possibility that with sufficient cycles of stress the vacancies present in equilibrium orient themselves into vacancy aggregates in a nonequilibrium fashion such as to accumulate at the crossings of dislocations, etc. This is the motivation for the present study. As an indication of the formation of these vacancy aggregates in the realistic case, we have chosen to study in some detail the activation energies of migration of vacancies in a distorted lattice represented by a dislocation "width".

II. THEORY

A. The Dislocation Model

The model of a dislocation chosen for the study of migration is of simple edge type in a face centered cubic lattice (see fig. 1). The (111) plane, a close packed plane, is taken as the slip plane. The total dislocation width is assumed finite and equal to twice the "width" which is given in the recent theory of Foreman, Jaswon, and Wood (ref. 1) as approximately eight atomic spacings (See Cottrell (ref. 2)). Lattice distortion is relaxed linearly in the direction parallel to that of slip from maximum distortion at the center of the dislocation width to no distortion at the edge of the dislocation width. Furthermore, the amount of distortion in planes parallel to the slip plane is taken as inversely proportional to the distance of the planes from the slip plane. Specifically, the amount of distortion is set equal to $K(\frac{1}{a})^{n}$, where K represents the distortion in the plane of atoms adjacent to the slip plane, and n ($n = 0, 1, 2 \ldots$) is an integer representing the number of the plane counted from the slip plane. Thus in the plane ($n = 0$) immediately adjacent to the slip plane the amount of distortion is K. For this particular study we set $a = 2$. The model, therefore, does not allow for the usual bending effect of a dislocation in a crystal lattice. It is hoped, however, that the dislocation model herein described represents those factors which would have most effect on the migration of vacancies.

B. Migration of a Vacancy in a Dislocation

In order to calculate the activation energies of migration of a vacancy in the dislocation a method similar to that of Bartlett and Dienes (ref. 3) is followed. For a certain direction of movement of the vacancy the potential of the atom with which the vacancy exchanges lattice positions is computed. Use is made of the Morse potential function,

$$U = D\left\{1 - \exp\left[-\alpha(r - r_0)\right]\right\}^2 ,$$

where U is the potential of the atom with respect to another atom at a distance r ; D and α are constants dependent on the solid involved; and r_0 is the equilibrium interatomic distance in the perfect lattice. For the computations which correspond to copper we take

$$r_0 = 2.55 \text{ A}$$
$$\alpha = 1.4 \text{ A}^{-1} .$$

Potentials are then given in the dimensionless form, U/D . For the potential of the moving atom the influence of the nearest neighbors to the two lattice sites occupied by the vacancy and the moving atom were considered. The potential of the moving atom at any point is then the sum of the potentials calculated with respect to each of the eighteen nearest neighbors. The effect of relaxation of neighbors is neglected as is also the effect of next to nearest neighbors.

As the atom moves between the two lattice sites, there are two points of minimum potential, hereafter referred to as relaxation points, and one point of maximum potential. The activation energy of migration is then the difference between the maximum potential and the appropriate one of the two relaxation potentials. The location of the points of relaxation and of maximum potential and the values of the potential at these points are determined by trial and error at various points on the straight line connecting the centers of the two lattice sites. Calculations off this straight line show little tendency for the atom to move along any other path.

The presence of the vacancy in the lattice affected the potential of more than just the moving atom, and the potentials computed considering only that atom gave results which were contradictory in one aspect. (See the later discussion in Section III.) In order to verify whether the vacancy tends, indeed, to migrate in the compressed half toward the center of the dislocation width, it would be necessary, in principle, to consider the potential of every atom of the lattice with respect to every other atom of the lattice, particularly those close to the vacancy. For the purpose of studying the direction of migration however, the potentials of three atoms occupying four lattice sites were computed and summed in the two cases schematically shown below. (Here X represents a lattice site occupied by an atom, and O, a lattice site occupied by a vacancy.)

	A	B		C	D	E
I	X	X	O	X	X	X
	A	B	C		D	E
II	X	X	X	O	X	X

The potentials of atoms A and E were not included in either case, since their potentials are not influenced by the presence of the vacancy considering the nearest neighbor approximation. Neither were the potentials of other nearest neighbor atoms off the path of motion included, as their effect merely enhances the previous result. Utilization of this generalized method resolves the contradiction, which will be discussed in Section III.

It was further interesting to determine, with one vacancy near the center of the distorted lattice, how close a second vacancy migrates toward it. In the case that the two vacancies are separated by two atoms, no single atom can be influenced by both vacancies in the nearest neighbor approximation. Therefore, it seems reasonable to assume that the second vacancy tends to migrate to a lattice site at least two atoms away from the first vacancy in a manner equivalent to that of the motion of the first vacancy toward the center of the dislocation width. To consider, however, the tendency of the second vacancy to migrate further, a method is used which is analogous to the generalized method in the previous case of an isolated vacancy. Three locations of the second vacancy relative to the first are considered:

	A	B		C	D		E	F
I	X	X	O	X	X	O	X	X
	A	B		C		D	E	F
II	X	X	O	X	O	X	X	X
	A	B			C	D	E	F
III	X	X	O	O	X	X	X	X .

The potentials of the atoms B, C, D, and E were computed, summed, and the sum compared in the three separate situations.

In these cases we considered only the relaxation potentials, and in each case the potentials of the four atoms were based on the influence of 72 nearest neighbors altogether.

III. RESULTS AND DISCUSSION

When calculations were made for an isolated vacancy considering only the potential of the moving atom along the path NM (see fig. 1), a series of independent curves were determined (see fig. 2), in which the ordinate represents the dimensionless potential, U/D , of the moving atom, and the abscissa gives the location of the moving atom with respect to the center of the dislocation width. Each of the curves containing one relative maximum represents a separate calculation. The positions and values of the maxima and minima on these curves were computed. The curves were then drawn in schematically through the computed points. For successive locations of the vacancy along the path NM from the edge of the dislocation width to the center (region of most dense atomic packing in the upper half) the values of the activation energies and of the relative maxima and minima are progressively smaller. This indicates that an atom with a vacancy next to it is more likely toward the center, whence vacancies are more likely nearer the center. However, it is seen that for each location with regard to the center, the moving atom at the left relaxation point has a lower potential than at the right relaxation point. This result, contrary to the overall results, seems to indicate a tendency for the vacancy to migrate away from the center of the dislocation width. When the generalized method discussed in Section II is applied, the relative values of the right and left relaxation potentials are reversed. The computations thus indicate that the vacancy tends to migrate to the more densely packed region of the dislocation as expected.

In studying the relaxation potentials involved in the migration of a second vacancy toward the first it was noted that the system had the minimum potential when the two vacancies were separated by two atoms, and the maximum when adjacent to one another forming a doublet vacancy. It seems then that there is little tendency for vacancies to form nonequilibrium doublets by this mechanism. The values of the potentials in the three cases are presented in Table I. Within the approximate model used here the values of cases I and II are about the same but case III is significantly higher.

A particular difficulty may be in evidence in this phase of the investigation, however, and it is not of such nature to permit a simple modification to the calculation. Since the calculation of the potential of an atom near two vacancies involved the summation of potentials over a greater number of neighboring atoms at larger distances than the analogous calculation for an atom near an isolated vacancy, it is possible that the effect of the nearer of the "nearest" neighbors to shield those at larger distances may be appreciable. If we take, however, this result at face value, it indicates that though "soft spots" may occur because of the motion of vacancies toward the center of the dislocation width, there is little tendency to form nonequilibrium vacancy doublets by the mechanism suggested here. Nevertheless, the "soft spots" formed as regions with higher nonequilibrium concentrations of vacancies may well be almost as effective in the initiation of a fatigue crack as regions of vacancy aggregates.

REFERENCES

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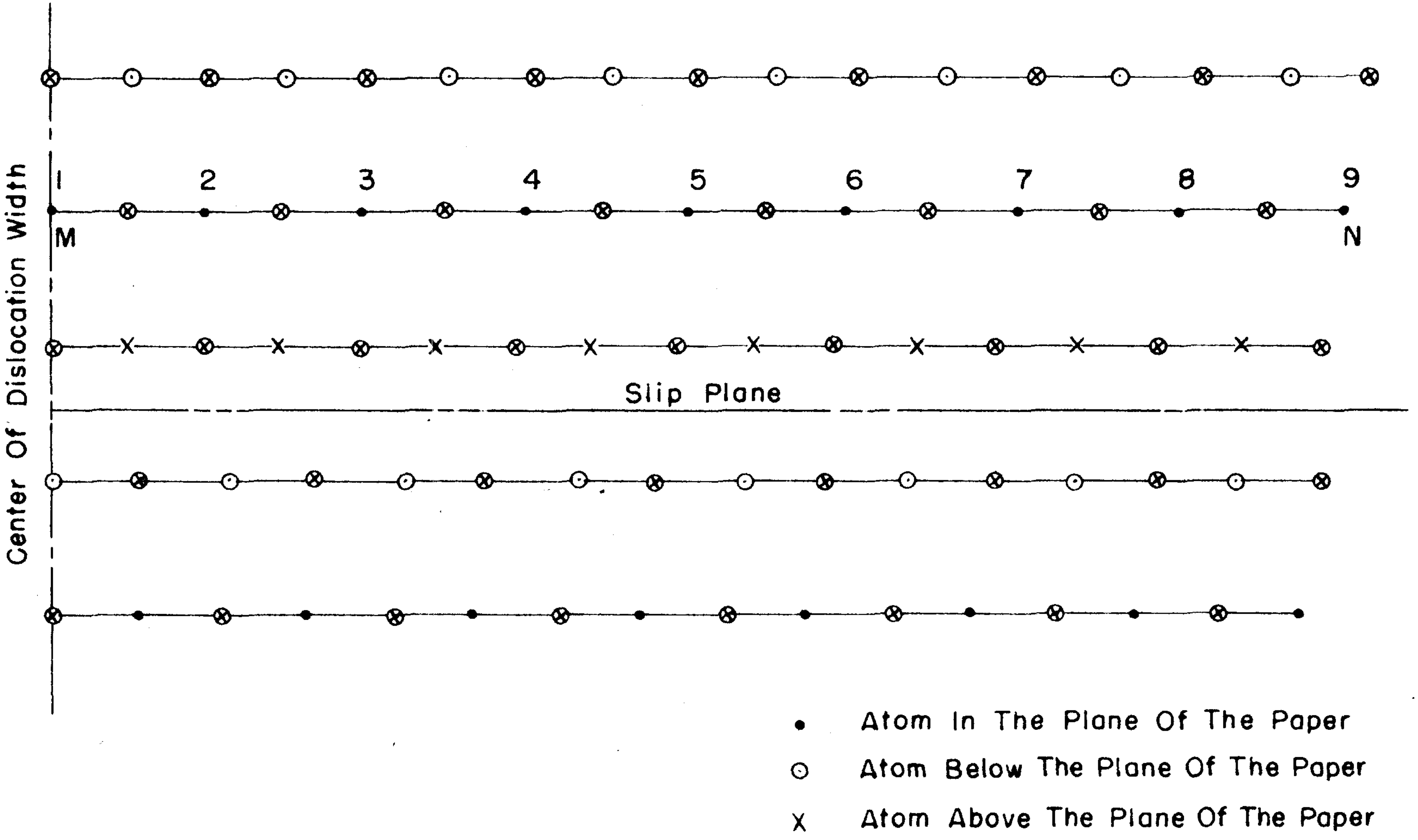

FIG. 1 — A VIEW OF THE LATTICE DISTORTED BY AN EDGE DISLOCATION

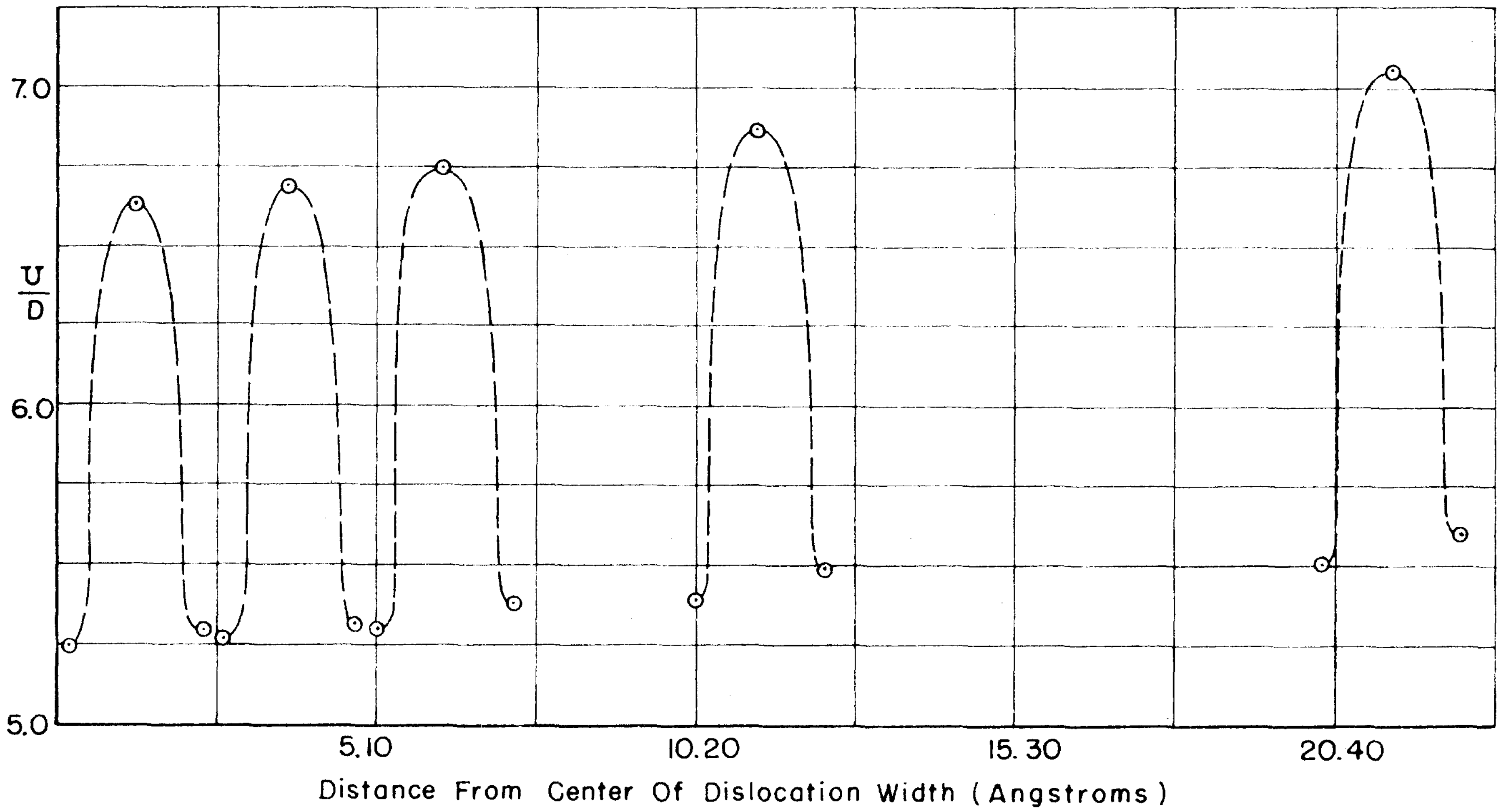

FIG. 2 - THE POTENTIAL OF THE MOVING ATOM FOR VARIOUS LOCATIONS OF A VACANCY

TABLE I.

RELAXATION POTENTIALS WITH TWO VACANCIES PRESENT IN VARIOUS LOCATIONS RELATIVE TO ONE ANOTHER

Case	Lattice Sites Occupied by Vacancies (fig. 1)	Potential (V/D)
I	2 and 5	21.40
II	2 and 4	21.67
III	2 and 3	22.75

APPENDIX

Sample Calculation

The detailed computation presented here is based on the motion of a vacancy from lattice site number 3 to site number 2 (see fig. 1). Therefore, the potentials computed are the potentials of the atom initially located in site number 2. Calculations then refer to each of the eighteen nearest neighbors of these two sites.

To compute the potential of the moving atom at the point of maximum potential an estimate is made of the location of this point along the line of centers between the two lattice sites. Knowing the Cartesian coordinates (x, y, z) of all lattice sites, the distance r, in Angstroms, from the assumed position to any nearest neighbor is then

$$r = \sqrt{(\Delta x)^2 + (\Delta y)^2 + (\Delta z)^2} .$$

In these computations the x direction is taken as the direction M to N (see fig. 1), and the y direction is in the plane of the paper. The origin was made to coincide with lattice site number 1. Assuming, then, the point of maximum potential to be at (3.653, 0, 0), we find the distance to the atom in site number 1, which has coordinates (0, 0, 0), to be

$$r = \sqrt{(3.653)^2} = 3.653 \text{ A} .$$

Then, we have that $r - r_o = 3.653 - 2.550 = 1.103$ A,

$$-\alpha (r - r_o) = -1.4(1.103) = -1.5442,$$

and $$e^{-\alpha(r-r_o)} = e^{-1.5442} = 0.2135 .$$

Finally, the dimensionless potential becomes

$$U/D = \left[1 - e^{-\alpha(r-r_0)}\right]^2 = \left[0.7865\right]^2 = 0.6186.$$

By computing the potential in this manner with respect to each of the eighteen nearest neighbors and summing, one arrives at the total potential of 6.6807.

Repeating this procedure as often as is necessary to locate the point of maximum potential, one finally finds the x coordinate of this point to be x = 3.683 A and the potential at that point to be 6.6889. The individual potentials and total potential for each of these locations and for the point x = 3.713 A are given in Table A-1.

Trial calculations are then made off the line of centers in each of the other two coordinate directions to determine if the path of motion is actually along the line of centers. For example, the same calculation as was made for the maximum potential point is again made at the two points: (3.683, 0.020, 0) and (3.683, -0.020, 0). The potentials at these two points were found to be 6.6946 and 6.6935 respectively. Similarly, computations made at the points (3.683, 0, 0.020) and (3.683, 0, -0.020) resulted in potential values of 3.6969 and 3.6952 respectively. Thus the value on the line of centers is seen to be a saddle point in the three-dimensional potential field and, as such, is the maximum potential attained by the atom in its motion between the two lattice sites.

In the same manner the two relaxation points are found to be (2.650, 0, 0) and (4.760, 0, 0) and the potentials at these points are 5.2651 and 5.3168 respectively.

After locating the relaxation points and point of maximum potential, the values of the potentials are rounded off to three significant figures as presented in the results. The comparison of the potentials in the two cases

		A	B		C	D	E
	I	X	X	O	X	X	X
		A	B	C		D	E
and	II	X	X	X	O	X	X

is made as follows:

I

a) The potential of the atom C is known from the previous calculation. At the right relaxation point it is 5.32.

b) The potential of the atom B is computed in its left relaxation point as though it were exchanging lattice sites with the vacancy. This computation again involves eighteen nearest neighbors although, in part, they are different neighbors than those considered previously. The potential thus computed is 5.25.

c) The potential of atom D is computed with respect to its twelve nearest neighbors but not permitting any relaxation. The value computed is 0.06.

d) The potentials of a, b, and c above are summed giving 10.63.

II

a) The potential of atom C is known from previous calculations to be 5.27 in its left relaxation point.

b) The potential of atom B is computed with respect to its twelve nearest neighbors, again not permitting relaxation. This value is 0.04.

c) The potential of atom D is computed in its right relaxation point as though it were moving to the vacancy location. The value computed is 5.38.

d) The sum of the three potentials for case II is 10.69.

Thus the potential of the system in configuration I is seen to be 0.06 less than that in configuration II.

TABLE A-1

POTENTIAL OF AN ATOM MIGRATING FROM LATTICE SITE NUMBER 2 TO SITE NUMBER 3 AT THREE TRIAL POINTS

Nearest Neighbor	Potential of Atom		
	(3.653, 0, 0)	(3.683, 0, 0)	(3.713, 0, 0)
A	0.3968	0.4110	0.4251
B	.0838	.0913	.0985
C	.3689	.3716	.3744
D	.1474	.1382	.1291
E	.5057	.4924	.4787
F	.6186	.6325	.6459
G	.4059	.4207	.4345
H	.4059	.4207	.4345
I	.3744	.3771	.3771
J	.3744	.3771	.3771
K	.4668	.4527	.4390
L	.4668	.4527	.4390
M	.6798	.6675	.6546
N	.4251	.4390	.4527
O	.1144	.1227	.1285
P	.3744	.3716	.3689
Q	.0866	.0797	.0730
R	.3850	.3704	.3556
Total	6.6807	6.6889	6.6862