

# Lawrence Berkeley National Laboratory

## Recent Work

### Title

ON THE THERMALLY ACTIVATED MOTION OF DISLOCATIONS

### Permalink

<https://escholarship.org/uc/item/366102nc>

### Author

Escaig, B.

### Publication Date

1969-10-01

*cy Z*

ON THE THERMALLY ACTIVATED MOTION OF DISLOCATIONS

RECEIVED  
LAWRENCE  
RADIATION LABORATORY

NOV 6 1969

B. Escaig

LIBRARY AND  
DOCUMENTS SECTION

October 1969

AEC Contract No. W-7405-eng-48

TWO-WEEK LOAN COPY

This is a Library Circulating Copy  
which may be borrowed for two weeks.  
For a personal retention copy, call  
Tech. Info. Division, Ext. 5545

LAWRENCE RADIATION LABORATORY  
UNIVERSITY of CALIFORNIA BERKELEY

*cy Z*

## **DISCLAIMER**

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

ON THE THERMALLY ACTIVATED MOTION OF DISLOCATIONS

B. Escaig<sup>\*</sup>

Inorganic Materials Research Division, Lawrence Radiation Laboratory,  
Department of Materials Science and Engineering, College of Engineering,  
University of California, Berkeley, California

\* Now in Laboratoire de Physique des Solides associe au C.N.R.S.  
91 - Orsay, France

The overcoming of an energy barrier by a dislocation segment is usually described by means of the general nucleation theory. As a result, the rate of the process is expressed as a function only of the maximum energy  $U$  of the barrier, through the well-known Arrhenius law  $\exp(-U/kT)$ . This short note is intended to show that in certain cases, the rate of overcoming of an energy barrier is not determined by the maximum energy, that is by the top of the barrier, but rather by the energy required by the first thermal events in starting the climb up the hill.

Let us first recall the fundamentals of the general nucleation theory<sup>(1)</sup>. The whole theory is the most simply described in its original context, phase nucleation. In order to reach a critical size, which has the maximum energy, embryos have to grow by addition of single atoms through a series of bimolecular equilibrium reactions:



where  $\alpha$  represents an atom of the phase  $\alpha$  and  $i$  is a cluster of  $i$   $\alpha$ -atoms. Notice here, that during a single thermal event, the nucleus energy increases from  $G(i - 1)$  to  $G(k)$ , so that the backward reaction  $i \rightarrow (i - 1) + \alpha$ , bringing the system to a lower energy, must be taken into account, in equilibrium with the forward reaction  $(i - 1) + \alpha$ . It has been shown that solving the whole set of such equilibriums yields a rate depending only on the top energy of the barrier through an Arrhenius type law.<sup>(2)</sup> This technique has been then extensively applied in solving a number of dislocation problems.<sup>(3)</sup>

Dealing with dislocation problems, little attention has been paid to the fact that in general the elementary thermal event does not bring the

nucleus size from  $i$  to  $i + 1$ . For example in dislocation loop shrinkage (or nucleation), decreasing the loop size  $x$  by one interatomic spacing  $b$  requires moving roughly  $x/b$  atoms. Let us assume a nucleus of size  $i$  is achieved. The next thermal event may correspond to a very different atomic configuration depending on whether (a) the nucleus size is starting to change from  $i$  to  $i + 1$ , or (b) from  $i$  to  $i - 1$ . Despite the fact that  $G(i - 1) < G(i) < G(i + 1)$ , it may occur in certain cases that the backward reaction  $i \rightarrow (i + 1) + \alpha$  is much more difficult to start than the forward reaction; it becomes practically negligible as compared with the forward reaction if the energy difference after the first thermal event, between configuration (a) and (b), is much larger than the thermal energy  $kT$ . In such a case, the whole preceding theory breaks down, since to reach the first unstable product, of size  $i^* + 1$  if  $i^*$  is the critical size, the set of successive equilibrium reactions (1) must now be replaced by a set of chain reactions:



As an illustrative example let us consider briefly the case of the shrinkage of triangular prismatic Frank loops, as produced by quenching and ageing in a face centered cubic metal. The Frank dislocation in low stacking fault f.c.c. metals splits, resulting in a truncated tetrahedron of stacking fault (Fig. 1). In order to shrink, the short stair rod segment at a corner, has to be dissociated into two attractive Shockleys, resulting in the formation of a new  $120^\circ$ -edge.<sup>(4)</sup> This nucleation can be described by an energy diagram  $G$  versus  $x$ , the length of the newly formed

edge expressed in spacings  $b$ , which shows an energy barrier, due to the stability of stair rods. To vary the length  $x$  by one  $b$ , a jog must be nucleated at the corner A, then propagated by diffusion along AB (Fig. 2). It is easy to see that nucleating a jog in order to start to change  $x$  in  $x + 1$  -- nucleation type (1) -- is much easier than doing the same to change  $x$  in  $x - 1$  -- nucleation type (2) --. Such a difference has been invoked to explain<sup>(5)</sup> in high stacking fault metals why prismatic loops grow in a polygonal shape (involving the type 2 of jog nucleation) and shrink in a round shape (type 1). Even a rough estimation, using the elastic dislocation theory, yields an energy difference between jog (2) and jog (1) of about  $\Delta U \approx \mu b^3/20 \approx 0.25\text{eV}$ , i.e. about as high as the usual jog formation energy. At an annealing temperature of  $400^\circ\text{C}$ , this means that the thermal probability for a jog of type (1) to be nucleated is about  $\exp(\Delta U/kT) \approx 100$  times higher than for type (2). Therefore the reverse reactions in this case can be neglected, resulting in a succession of chain reactions as in equation (2).

Such a set of reactions is easily solved. To assure no accumulation in any reaction products all the reaction rates must be equal under steady state conditions, i.e.:

$$k_1 [1] = \dots = k_i [i] = k_{i^*} [i^*] = v$$

where  $[i]$  is the concentration of  $i$ -sized nuclei, and  $k_i$  is the rate constant of the reaction  $\alpha + i \rightarrow i + 1$ . Assuming a thermal equilibrium between all the intermediate thermal events from  $i$  to  $i + 1$ , yields  $k_i \propto \exp(-\Delta G_i/kT)$ ,  $\Delta G_i = G(i + 1) - G(i)$ . This means that a higher step  $\Delta G_n$ , or a lower  $k_n$ , induces an accumulation of nuclei  $n$ , or a higher  $[n]$  until compensation takes place in order to keep constant the product

$k_n \cdot [n]$ . The production rate of final product, that is the rate of the whole process is given by

$$v = [1] \exp(-\Delta G_1 / kT)$$

where  $[1]$  is the initial concentration of defects and  $\Delta G_1$  is the height  $G(2) - G(1)$  of the first step. Obviously if the process involves a non-conservative motion of dislocations, i.e. if vacancies are created or annihilated, the self diffusion energy  $U_D$  must be added in the activation energy as usual<sup>(2)</sup>, giving as the rate controlling activation energy:

$$G = U_D + \Delta G_1$$

More generally, it is possible to consider a less extreme case. Let us assume that the reverse reactions do occur only until some nucleus size  $y$ :



The usual nucleation theory yields  $[y] = [1] \exp(-G(y)/kT)$ , and the preceding considerations give as the rate of nucleation:

$$v = [y] \exp(-\Delta G_y / kT) = [1] \exp(-G(y + 1)/kT)$$

From this equation it is clear that our result differs from the usual nucleation theory only in assuming  $y + 1 < i^*$  instead of  $y + 1 = i^*$ , i.e. that the reverse reactions may become difficult at some stage before the maximum energy size is reached.

Concerning the shrinkage of Frank loops, it is hard to rule out completely the possibility of reverse reactions in the very first steps. For example, for a new edge length  $l = b$ , or  $x = 1$ , the reverse reaction



gives back the fully dissociated truncated tetrahedron (Fig. 1). For  $y = 1, 2$  or  $3$  it is necessary to evaluate how much energy is gained in recombining more or less the attractive Shockleys into stair-rods. However, the maximum energy configuration is reached at a stage far beyond these first few steps. Therefore, the activation energy is expected to be much less than the maximum energy of the barrier. More precise computations<sup>(6)</sup> show that only this theory can explain the observed shrinkage of Frank loops in silver,<sup>(7)</sup> a metal of low stacking fault energy. A similar explanation could account for the collapse of stacking fault tetrahedra.<sup>(6)</sup> The problem of the nucleation rate of dislocation loops in quenched metals, still unexplained,<sup>(8)</sup> will be studied in a separate publication along the same line.

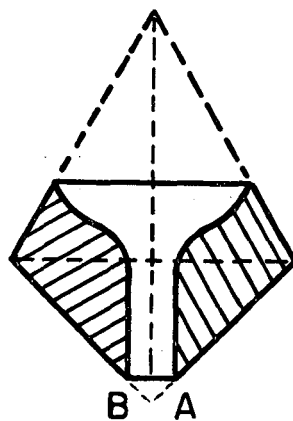
In summary, it is thought that such a modification of the nucleation theory could be useful in numerous dislocation problems. It is emphasized that the rate controlling activation energy of an activated process should not always be identified with the maximum energy of the barrier. Rather it may correspond to the first step or the first few steps up the barrier in cases where the reverse reaction, going down the hill, contains difficult steps compared to any of the forward steps that lead up the hill.

#### A C K N O W L E D G E M E N T S

It is a pleasure of the author to thank Professor J. Washburn and Professor J. P. Mirth for helpful discussions. The support of this work by the United States Atomic Energy Commission, through the Inorganic Materials Research Division of the Lawrence Radiation Laboratory is gratefully acknowledged.

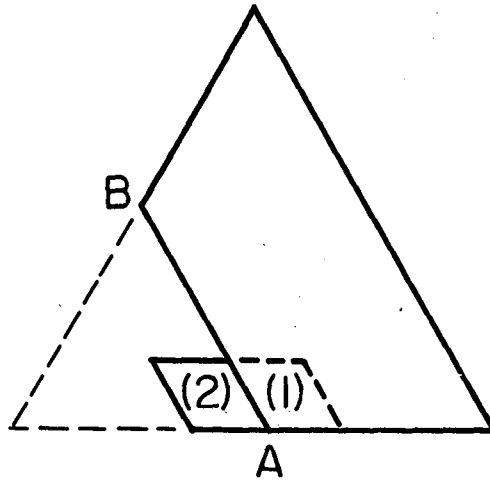
REFERENCES

- (1) M. Volmer, Kinetic der Phasenbildung, Julius Springer Verlag, Dresden, (1939). Also J. P. Hirth and G. M. Pound, Condensation and Evaporation, Perg. Press, Oxford, (1964); D. Turnbull, Solid State Phys., 3, 225 (1956).
- (2) D. Turnbull and J. C. Fisher, J. Chem. Phys., 17, 1, 71 (1949).
- (3) J. P. Hirth and J. Lothe, Theory of Dislocations, McGraw-Hill, p. 490, 560 (1968).
- (4) M. J. Yokota and J. Washburn, Phil. Mag., 16, 459 (1967), also J. Washburn and M. J. Yokota, J. Cryst. Latt. Defects, 1 (1969).
- (5) J. Silcox and M. J. Whelan, Phil. Mag., 5, 1 (1960).
- (6) B. Escaig, to be published
- (7) R. E. Smallman, P. S. Dobson, P. J. Goodhew, Proceedings of the Int. Conf. on The Strength of Metals and Alloys, Tokyo 1967, in Trans. of the Jap. Inst. of Metals, 9, 562 (1968).
- (8) T. L. Davis and J. P. Hirth, J. Appl. Phys., 37, 5, 2112 (1966).



XBL699-3799

Fig. 1 New  $120^\circ$  edge, AB, on a dissociated Frank loop



**XBL699 - 3800**

Fig. 2 The two kinds of jogs nucleated at corner A

LEGAL NOTICE

*This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:*

- A. Makes any warranty or representation, expressed or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or*
- B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.*

*As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.*

TECHNICAL INFORMATION DIVISION  
LAWRENCE RADIATION LABORATORY  
UNIVERSITY OF CALIFORNIA  
BERKELEY, CALIFORNIA 94720