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UCRL-10390

UNIVERSITY OF CALIFORNIA
Lawrence Radiation Laboratory
Berkeley, California

Contract No. W-7405-eng-48

ON THE STABILITY OF QUENCHED LOOPS IN FACE-CENTERED CUBIC METALS

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August 1962

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Abstract

The stability of quenched Frank sessile loops with respect to perfect prismatic loops is studied on a new model. It is concluded that measurement of the size of stacking fault rings does not give the right value for the stacking fault energy. The occurrence of stacking fault defects is predicted for metals with relatively high stacking fault energy like aluminum. Experiments to check the theory are proposed.

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1. Introduction

Observations of thin films of quenched face-centered cubic metals have revealed several large defects[1]: perfect prismatic dislocation loops, Frank sessile loops surrounding a stacking fault, tetrahedra. Helical dislocations have been observed in alloys[2].

Although the existence, the geometrical features and some mechanisms by which they can transform into each other have been predicted or explained quite accurately[1, 3-7], very little is known of the reasons for which a given defect is observed rather than another one.

Therefore, it is the purpose of this paper to study theoretically the stability of a Frank sessile loop with respect to a perfect prismatic loop by assuming they can transform into each other by a glide mechanism[7, 8].

The next paragraph of this paper will be devoted to the description of our model and of its general consequences. In the third paragraph we shall apply the results of our calculation to the description of the experimental situation in face-centered metals. We shall show that previous determinations of the stacking fault energies in the metals based upon the determination of the size of quenched loops are not reliable[9]. We shall compare our results to those obtained by Czjzek, Seeger and Mader[10] in a similar work on the transformation of Frank sessile loops into tetrahedra and make some remarks on the processes of formation of quenched-in dislocation loops.

2. Model

Let us consider a Frank sessile loop (F), with Burgers vector $\vec{b}_F = \frac{a}{3} \langle 111 \rangle$, lying in the (111) plane (Q) (Fig. 1). Kuhlmann Wilsdorf[7]

has suggested that a Shockley partial (S) with Burgers vector $\vec{b}_s = \frac{a}{6} \langle 11\bar{2} \rangle$, able to glide in the plane (P), can be nucleated inside the loop, develop under the effect of the stacking fault energy, sweep the stacking fault, and recombine with the Frank sessile dislocation giving a perfect prismatic dislocation (P) through the reaction

$$\vec{b}_F + \vec{b}_s = \vec{b}$$

which can be written

$$\frac{a}{3} \langle 111 \rangle + \frac{a}{6} \langle 11\bar{2} \rangle = \frac{a}{2} \langle 110 \rangle$$

$\vec{b}$, being the Burgers vector of the perfect dislocation and a, the lattice parameter.

We shall examine this process in detail. The Burgers vectors of the loops (S) and (F) are perpendicular, which allows us to neglect their elastic interaction[11]. Therefore, the loop is subjected to two forces: its line tension, which tends to shrink it, and the stacking fault energy which tends to develop it. If we assume that both stresses are isotropic, the equilibrium shape of the Shockley partial will be circular.

We assume now that the Frank sessile loop is circular. We shall show in our appendix that this assumption does not restrict the validity of our conclusions. From the preceding remarks it results that the place where the Shockley partial is nucleated is irrelevant.[8] We shall, therefore, place it at the center of the Frank sessile loop.

Let us examine at first the energy necessary for the nucleation of the Shockley partial (S), that is the energy necessary to create a Shockley partial of radius b_o, b_o being the core radius. Since $b_s < b_o < 2b_s$[11], the creation of such a loop involves the motion of few atoms in the region

of the core. Moreover, the strain energy of such a small loop is very low. Therefore, we can say that the energy for the nucleation of the loop (S) is small.

For example, if we take $b_o = 2b_s$ and if we use for the line tension[11] the overestimated value of $.5Gb^2$, we get for the activation energy 5eV. Therefore, it is not unreasonable to assume that the energy necessary to nucleate (S) is of the order of one or two electron volts. In all our further discussion we shall neglect the nucleation process.

We shall now study the propagation of the loop (S). For this we will make use of the notations of Fig. 1 and calculate the total energy of the configuration, taking the zero level of energy when the radius r of the Shockley partial is equal to b_o. The energy will be the algebraic sum of a line energy and of the surface energy

$$W = \frac{Gb_s^2}{4\pi K} 2\pi r \operatorname{Log} \frac{r}{b_o} - \pi r^2 \gamma + \pi b^2{}_o \gamma \qquad (1)$$

where G is the Young modulus, γ is the stacking fault energy, K is a constant lying between $1 - \nu$ and 1 and related to the character screw or edge of the dislocation, and ν is the Poisson ratio.

Introducing K in formula (1) is indeed contradictory with the assumption that the line tension is isotropic. K, however, varies for FCC metals between .65 and 1. The validity of our calculation is not restricted if we choose for K an average value of the order of 0.8. By setting

$$\gamma_c = \frac{Gb_s^2}{4\pi K b_o} \qquad (2)$$

and

$$W_o = \pi b_o^2 \gamma_c \tag{3}$$

we can write (1) as

$$W = W_o \left(\frac{2r}{b_o} \operatorname{Log} \frac{r}{b_o} - \frac{\gamma}{\gamma_c} \frac{r^2}{b_o^2} + \frac{\gamma}{\gamma_c}\right). \tag{1'}$$

In order to know whether or not the loop (S) will expand, we must take the derivative $\frac{dW}{dr}$ and study its sign

$$\frac{dW}{dr} = 2W_o \left(\operatorname{Log} \frac{er}{b_o} - \frac{\gamma r}{\gamma_c b_o}\right). \tag{4}$$

Before studying this equation mathematically let us remark first that our analysis applies as well to the transformation of a perfect prismatic dislocation loop into a Frank sessile loop by splitting of the perfect dislocation into a Shockley partial and a Frank sessile[8].

(a) If $\gamma \geqslant \gamma_c$, $\frac{dW}{dr}$ is never positive. The energy decreases when the Shockley partial grows. This means that only perfect dislocation loops are stable in such metals. If a Frank sessile existed in such a metal, its transformation into a perfect loop would need only the small activation energy necessary to nucleate a Shockley partial.

The numerical value of γ_c cannot be calculated accurately because it depends on b_o which is unknown. As said previously

$$b_s \lesssim b_o \lesssim 2b_s \tag{5}$$

and therefore from formula (2)

$$\gamma_c = (4.5 \pm 1.5)\ 10^{-2} Gb \tag{6}$$

From formulas (2) and (6) one can easily see that γ_c is of the order of magnitude of the stacking fault energy γ_m of a metal in which dissociated dislocations are one Burgers vector length wide.

More precisely $\gamma_c = \frac{\gamma_m b}{b_o}$ i. e., $.85\gamma_m \lesssim \gamma_c \lesssim 1.7\gamma_m$. Therefore, it is not likely that metals can have a stacking fault energy larger than γ_c.

(b) If $\gamma < \gamma_c$, $\frac{dW}{dr}$ is at first positive and then negative. Therefore as a function of r, W increases until r reaches the value r_c, and then decreases monotonically until it is equal to 0 when $r = R_c$ (Fig. 2). The transformation is only possible through an activation energy W_M. W_M is represented in Fig. 3 as a function of the ratio γ/γ_c.

By calculating W_o through equations 2, 3 and 5 one gets

$$W_o = (.15 \pm .05)\, Gb^3 \simeq 1\text{eV}. \tag{7}$$

By looking at Fig. 3 one sees that W_M increases smoothly when γ decreases from γ_c to $.4\gamma_c$ and increases very rapidly when γ decreases from $.4\gamma_c$ to 0.

This means that for metals with low stacking fault energy ($\gamma \lesssim .4\gamma_c$) the activation energy W_M is very high, and for metals with intermediate stacking fault energy ($.4\gamma_c \lesssim \gamma < \gamma_c$) the activation energy is quite low, of the order of 1eV.

We can now discuss the stability of the loops with respect to their size R^*. For this purpose we have represented in Fig. 4 the variation of r_c and R_c as a function of γ/γ_c. They divide the plan into three regions a, b, and c. We have drawn a line corresponding to $R \simeq 50$Å corresponding to the minimum radius of the loops which can actually be observed by electron microscopy. We remark that this line cuts both $r_c[\frac{\gamma}{\gamma_c}]$ and

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*R determines the maximum value of r.

$R_c[\frac{\gamma}{\gamma_c}]$ for values of γ smaller than $.4\gamma_c$.

We shall consider three cases:

First case

$$R < r_c \qquad \text{Region a}$$

The stable configuration is still the Frank sessile loop.

Second case

$$r_c < R < R_c \qquad \text{Region b}$$

The stable configuration is still the Frank sessile loop. However, the transformation of a perfect prismatic loop into a Frank sessile needs an activation energy which is quite low for metals with intermediate stacking fault energies ($.4\gamma_c \lesssim \gamma \lesssim \gamma_c$) and quite high for metals with low stacking fault energies ($\gamma \lesssim .4\gamma_c$).

In fact, loops lying in this region can only be observed in metals with low stacking fault energy ($\gamma < .4\gamma_c$).

Third case

$$R > R_c \qquad \text{Region c}$$

The stable configuration is the perfect prismatic loop. However, the transformation of a Frank sessile loop into a perfect prismatic loop needs an activation energy W_M which can be very high for metals with low stacking fault energies and reasonable for metals with intermediate stacking fault energies.

3. Comparison with experiment

The behavior of dislocations in face-centered cubic metals has been shown to be closely related to the value of the stacking fault energy γ in these metals[11, 12]. Therefore it is of great importance to know accurately the latter quantity. Unfortunately, as a result of the great

difficulty of making direct measurements, the figures found in the literature give widely scattered values of γ. For pure copper, for example, we find measured values of γ varying from 40 ergs. cm^{-2} [13] to 170 ergs. cm^{-2} [9].

We shall discuss in this paragraph the accuracy of the method for estimation of stacking fault energy which consists of measuring the size of quenched loops in face-centered cubic metals.

We can conclude from the analysis done in paragraph two that metals in which Frank sessile loops are observed have a stacking fault energy γ lower than the critical value γ_c. This is the case of gold, silver, copper[1] and aluminum[14]. We give in Table 1 the values of γ_c calculated from formula 2.

Table 1

Values of γ_c for usual FCC metals

	Au	Ag	Cu	Al	Ni	Pt
γ_c ergs. cm^{-2} within 40%	360	390	550	350	860	780

These values are indeed much larger than values quoted in the literature.

Nothing more precise about the stacking fault energy can be concluded from the measurement of the radius of the Frank sessile loops. This results from the fact that metastable loops of both types can be observed. Therefore, previous estimates of γ based on this method are not accurate.

Before discussing in detail the situation for each metal, we shall make some remarks on the formation of the loops.

In metals with stacking fault energies lower than γ_c, the discs of vacancies lying in (111) planes probably coalesce into Frank sessile loops, and grow as Frank sessile loops. When they are large enough they can transform into perfect prismatic loops needing an activation energy W_M. As shown previously W_M is small for metals for which $.4\gamma_c \lesssim \gamma < \gamma_c$ and large in metals for which $\gamma \lesssim .4\gamma_c$. In that case, the Frank sessile loops will not transform into perfect prismatic loops. Therefore, such loops can be obtained either by the breaking of a helix or by coalescence of a disc of vacancies lying in a plane different from (111). In both cases the loops can rotate toward the (111) plane.

If we start with such a perfect prismatic loop lying in the (111) plane we can say that it is stable when its radius is large enough ($R > R_c$). If we anneal it, it shrinks and, while its radius decreases, it becomes at first metastable then transforms spontaneously into a Frank sessile loop.

The measure of the critical radius at which the transformation occurs gives a good estimate of the activation energy for perfect loops lying in the (111) plane. When $\gamma > .4\gamma_c$, the critical radius is very small and, therefore, if observed during annealing in the microscope, such loops will become too small to observe before transformation. If $\gamma < .4\gamma_c$ the transformation will occur for an observable value of the radius. Moreover, the activation energy W_M is so high that we can neglect the transformations occurring in the metastable zone.

Let us now consider each case in detail.

<u>Aluminum</u> For a long time only perfect prismatic loops have been observed in this metal[1]. More recently Frank sessile loops have

been observed in very pure aluminum[14]. This suggests (a) that the stacking fault energy of aluminum is smaller than γ_c, (b) that other factors than the stacking fault energy play a role in determining the type of loop that is formed (impurity content for example), (c) annealing experiments on very pure aluminum should at least show whether or not the stacking fault energy γ_{Al} is higher than $.4\gamma_c$. Such experiments have been performed with less pure aluminum[15]. No transformation was observed which suggests that

$$140 \text{ ergs. cm}^{-2} < \gamma_{Al} < 350 \text{ ergs. cm}^{-2}$$

Copper Both perfect and imperfect dislocations have been observed in this metal[1]. Annealing experiments should provide some information on the value of the stacking fault energy.

Silver Perfect and imperfect loops[1] and tetrahedra[16] have been observed in silver. From a study similar to ours done by Czjzek, Seeger and Mader[10] we can conclude that the stacking fault energy of a metal, in which tetrahedra are observed, is lower than $\gamma_c \simeq 2 \times 10^{-2}$ Gb.

Since this value is of the order of $.4\gamma_c$, annealing experiments of the perfect loops lying in the (111) planes must probably allow us to actually observe the transformation of perfect loops into Frank sessile loops and therefore to have a good estimate of the stacking fault energy of silver. Nothing more can be said at the moment about the other FCC metals.

Appendix

1. Propagation of a Shockley partial which has been nucleated at a corner of a triangular Frank sessile loop (F).

The purpose of this first section is to show on a very rough model that the orders of magnitude of the quantities calculated in part 2 of our paper are not dependent upon the geometry used.

We therefore suppose that a Shockley partial (S) has been nucleated at a corner (A) of an equilateral triangle shaped Frank sessile (F) (Fig. 5a). The Burgers vectors $\vec{b}_S$ and $\vec{b}_F$ are perpendicular. Therefore the equilibrium shape of the loop is a portion of circle tangent at (N) and (P) to the sides of the triangle and we look at its propagation in the same way as we did in section 2 of our paper. The main difficulty in calculating the total energy comes from the fact that we now have to calculate the energy of the irregularly shaped ANPA dislocation loop. We shall therefore make the assumption that the line tension is no different than the line tension of a circular loop which is quite rough but must not change the order of magnitude of the result.

With the same notation as in section 2 of our paper and with the same conventions for the zero energy level we calculate the total energy (W)

$$W' = W'_o \left(2r \operatorname{Log} \frac{r}{b_o} - \frac{\gamma}{\gamma_c} \frac{r^2}{b_o^2} + \frac{\gamma}{\gamma_c}\right)$$

with

$$W'_o = \left(\frac{2}{3} + \frac{3}{\pi}\right) W_o \simeq 1.17\, W_o$$

By comparing these equations to equations (1') and (3), it is obvious that the only results which are changed are related to the total energy (W)

which is increased by less than 20%. Therefore the main conclusions of our paper are not changed in this case.

2. Propagation of a Shockley partial toward the corners of an equilateral triangle shaped dislocation.

Suppose that a Shockley partial has been nucleated at the center O of a stacking fault triangle (F) and that it has grown to become tangent to the sides of the triangle in MNP (Fig. 5b). Let us assume that a further step is represented by the situation P'P"M'M"N'N"P'. The segments like N'P' are supposed to be circular and tangent to the sides of the triangle.

We shall now calculate the energy necessary for the sweeping of the total area by the Shockley partial. To do this we shall use besides the assumptions of part 2 of our paper the following assumption: the line tension τ of the loop P'P"M'M"N'N"P' is constant and equal to the line tension of the loop PMN. We shall take the zero level for the energy when the Shockley partial is in the position PMN with radius $\frac{l\sqrt{3}}{6}$, where l is the length of the side of the triangle.

The energy is then

$$W = (3\sqrt{3} - \pi)\left[(\gamma r^2 - 2\tau r) + \frac{\tau l}{\sqrt{3}} - \frac{\gamma l^2}{12}\right]$$

One sees that in order to reach the corners of the triangle, the Shockley partial must overcome a potential barrier of the order of $\Delta W = -W(r_c)$, where $r_c = \frac{\tau}{\gamma}$.

With loops of reasonable size ($l \simeq 150$Å) the potential barrier can be shown to be of the order of 5eV for metals with high stacking fault energy and can be as high as 50eV for metals with low stacking fault energy.

Therefore, it is not likely that triangular shaped loops can be transformed into perfect loops by a simple glide process.

Figure Captions

Fig. 1 Model used for the calculation of paragraph 2

Fig. 2 Plot of the energy versus the radius of the Shockley partial dislocation

Fig. 3 Plot of the activation energy W_M versus the stacking fault energy (arbitrary units W_o and γ_c)

Fig. 4 Plot of the critical radius r_c and R_c versus the stacking fault energy (arbitrary units)

Fig. 5a Model used for the calculation of appendix 1

Fig. 5b Model used for the calculation of appendix 2

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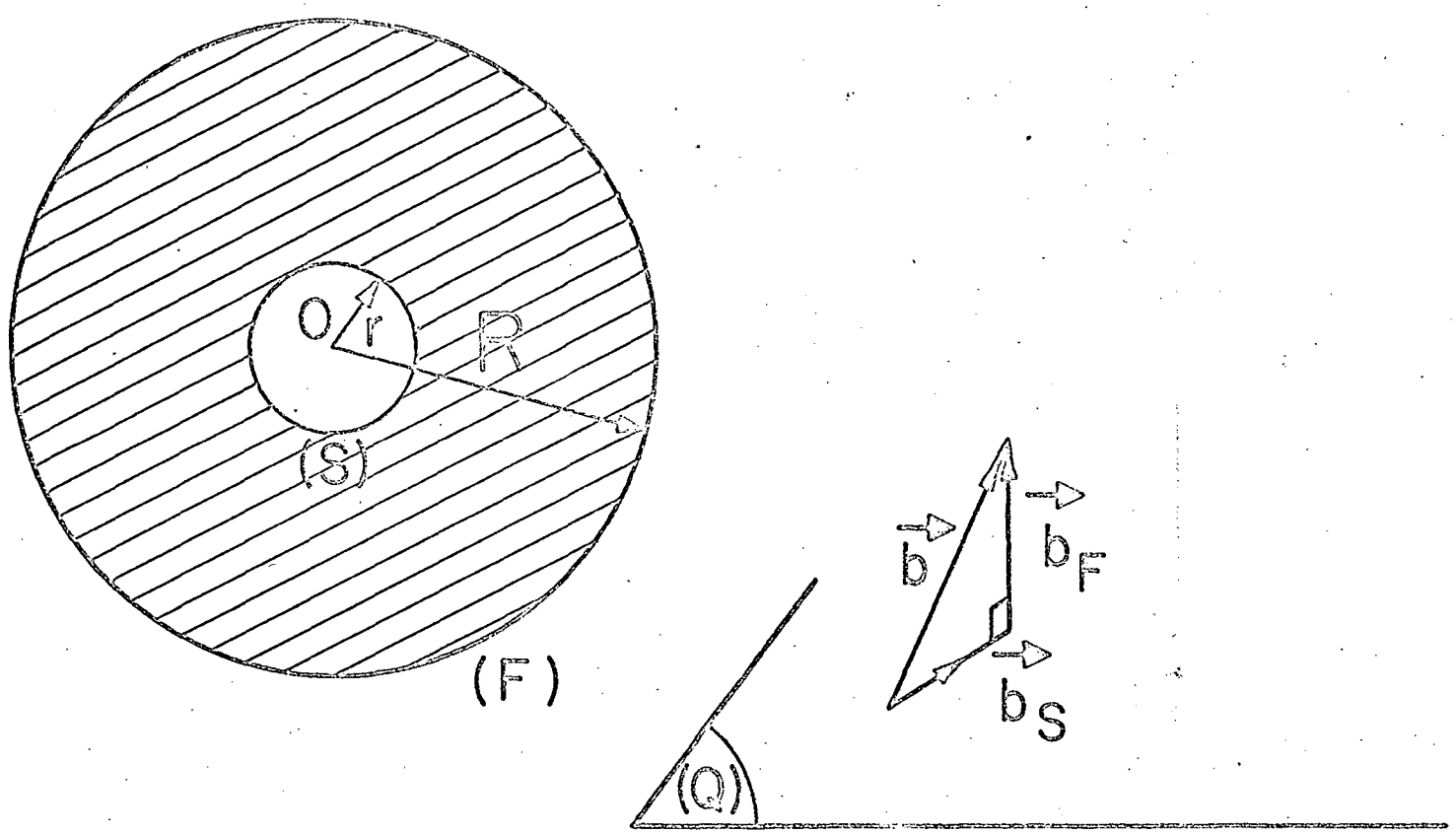

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Fig. 1

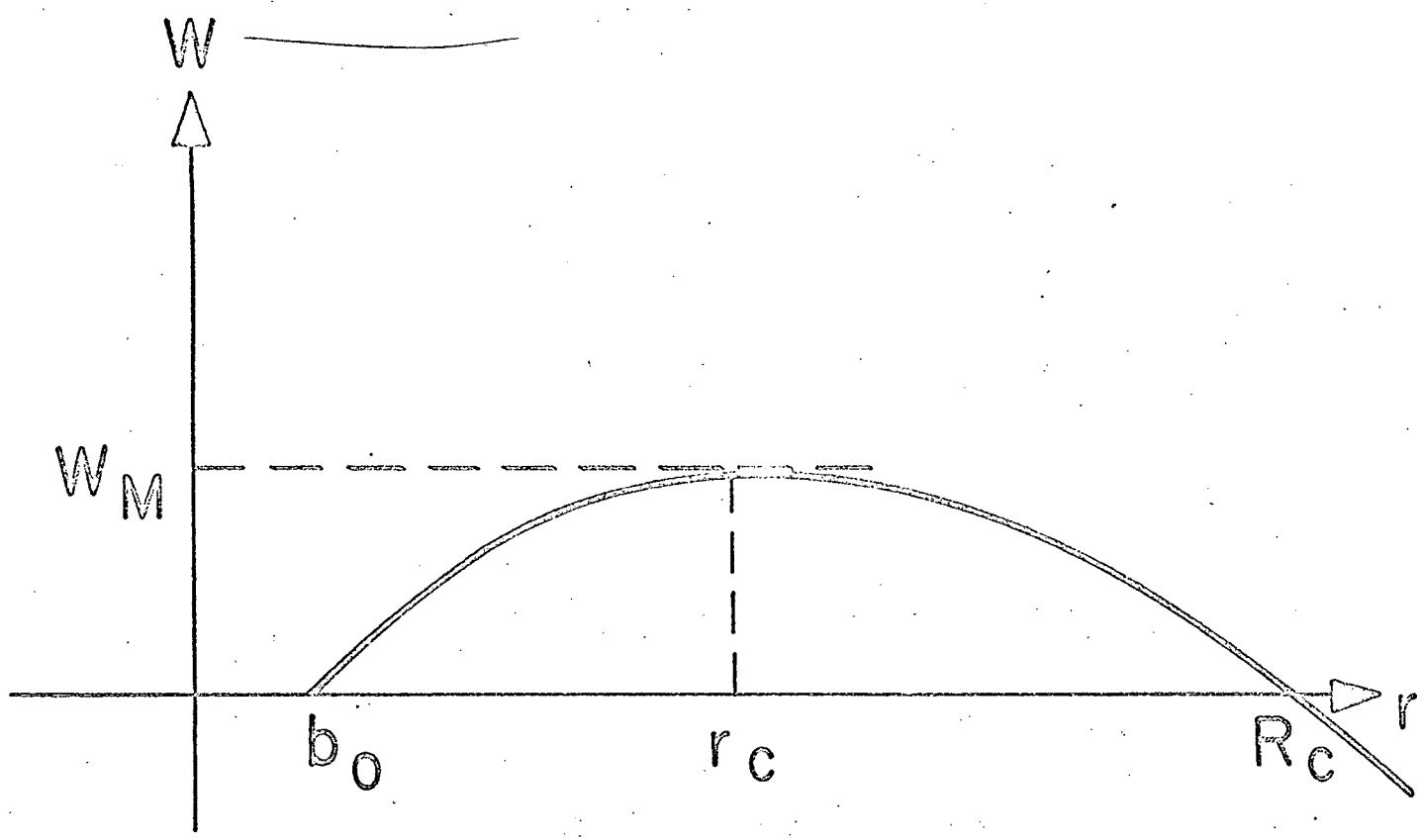

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Fig 2

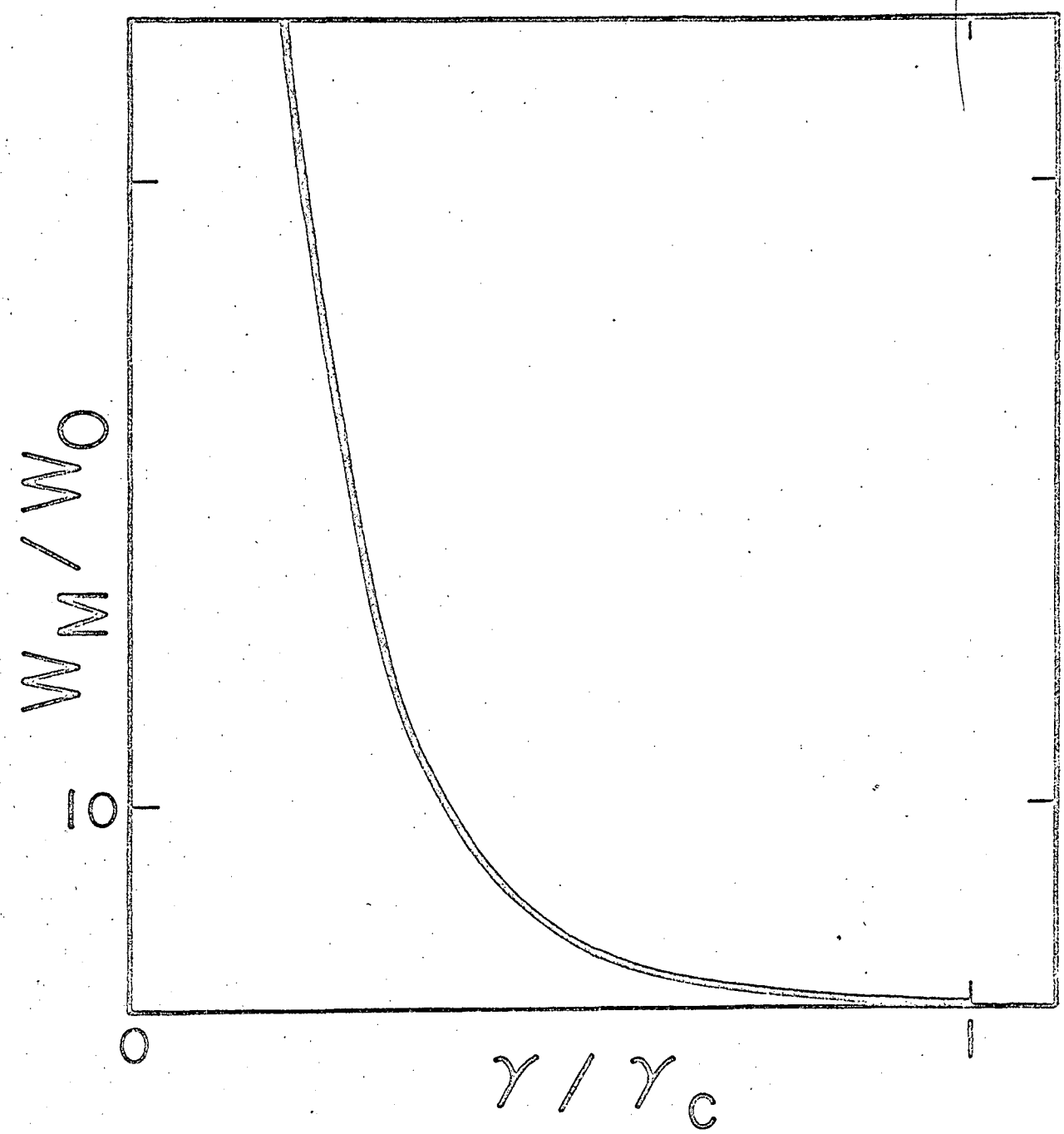

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Fig. 3

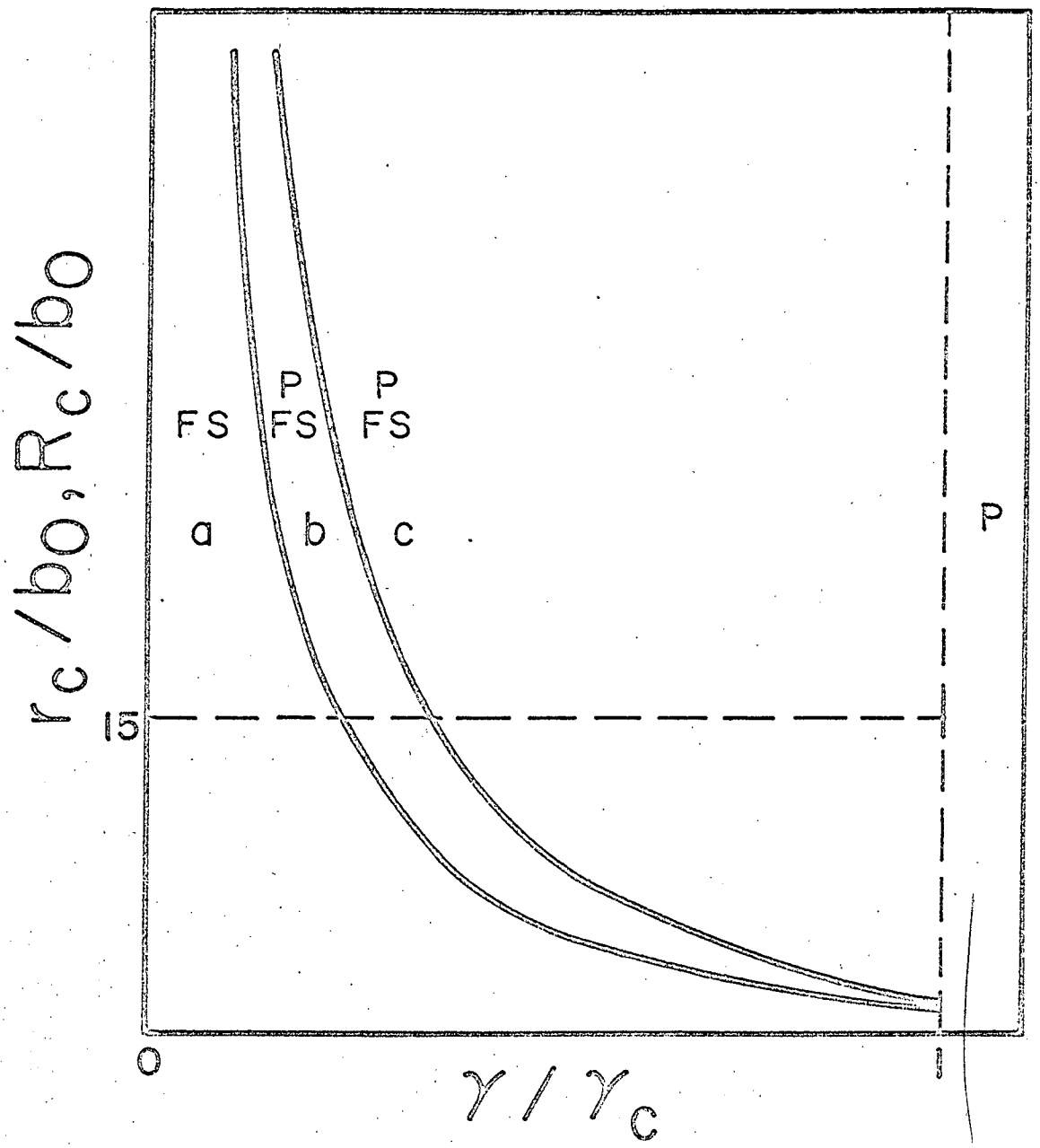

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Fig. 4

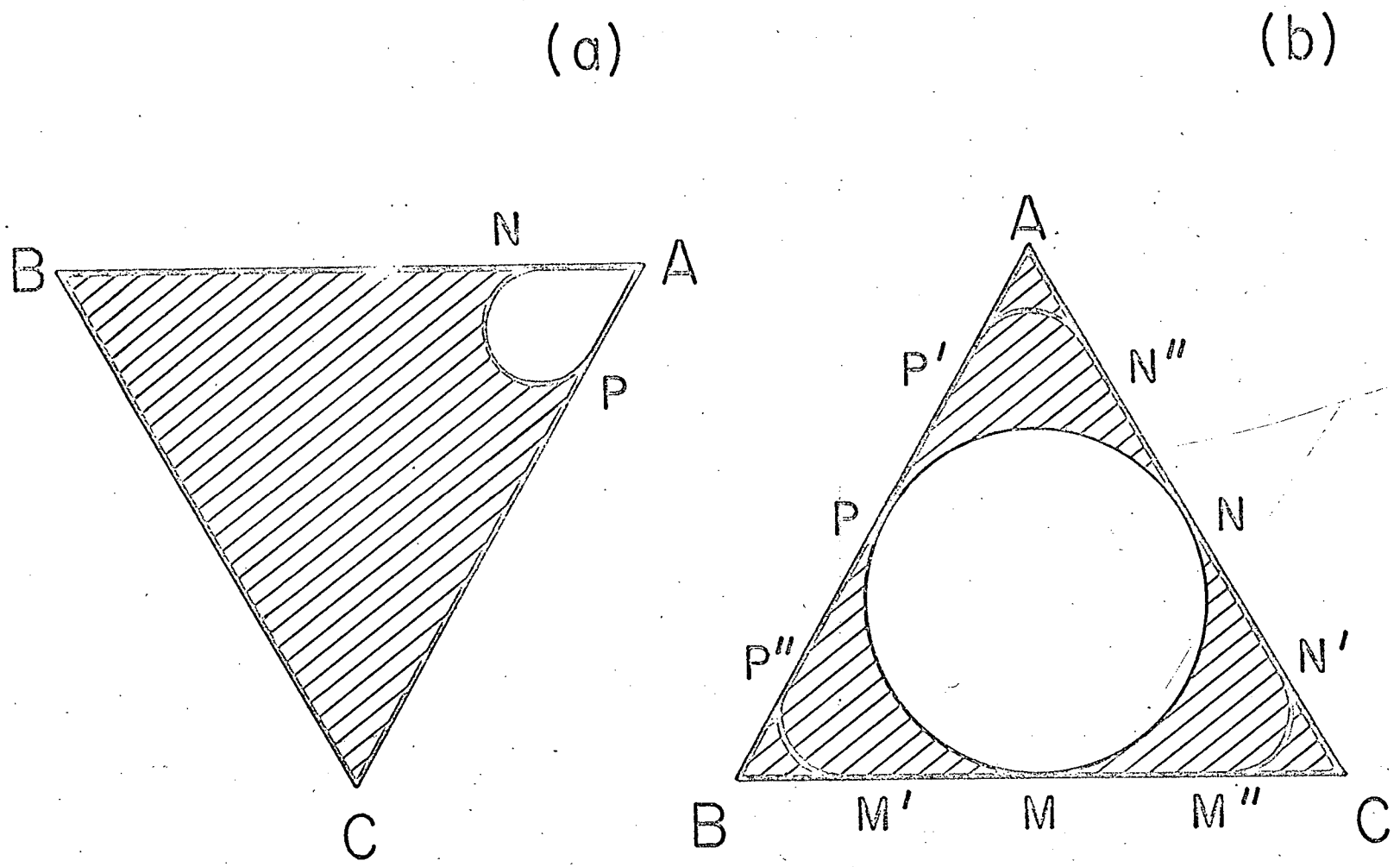

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Fig. 5