UCRL-17293

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CAMEL-HUMPS PEIERLS HILLS IN IRON

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Submitted to Acta Metallurgica UCRL-17293

UNIVERSITY OF CALIFORNIA

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AEC Contract No. W-7405-eng-48

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Recently, Chang and Graham[1] calculated the Peierls hills for an edge [111] dislocation lying in the (110) plane in Fe. They used relaxation techniques with a two atom anhormonic interaction potential so adjusted as to give the known second and third order elastic properties of Fe. ΔE, the energy per identity distance along such straight dislocation, is plotted in Fig. 1 versus the distance moved in the y direction; the hills have two equal peaks and primary and secondary minima. If $\Gamma(y)$ is the line tension of the dislocation, periodic in the y direction with a period equal to the Burgers vector $b = 1/2[111]$, the plot can be analytically fitted by the equation

$$\Gamma(y) = \frac{\Gamma c+\Gamma o}{2} + \frac{\Gamma c-\Gamma o}{2}\left(\frac{\alpha}{4} + \cos\frac{2\pi y}{b} - \frac{\alpha}{4}\cos\frac{4\pi y}{b}\right) \qquad (1)$$

with $\Delta E = (\Gamma(y) - \Gamma o)\, 2\sqrt{2}\, b$, and $\alpha = 3.865$, $\Gamma(y) = \Gamma o$ at $y = 0$, $\Gamma(y) = \Gamma c$ at $y = b/2$. More generally, for $\alpha > 1$, such an equation represents camel-hump types of hills. Γm, the maximum value of $\Gamma(y)$, is related to Γo and Γc by the relation:

$$\Gamma c = \frac{2\Gamma m - \Gamma o\left(1 - \frac{1}{2\alpha} - \frac{\alpha}{2}\right)}{1 + \frac{1}{2\alpha} + \frac{\alpha}{2}} \qquad (2)$$

On the basis of the Dorn-Rajnak theory,[2] the kink energy under zero stress, U_K, and the energy to nucleate a pair of kinks on a perfect dislocation moving beyond the hills under an applied stress τ^*, U_n, are given by

$$U_K = \Gamma o \int_{-b/2}^{+b/2} \{\frac{\Gamma(y)}{\Gamma o} - 1\}^{1/2} dy \tag{3}$$

$$U_n = 2 \int_{yo}^{yc} \{\Gamma(y)^2 - [\tau^* b(y-yo) + \Gamma(yo)]^2\}^{1/2} dy \tag{4}$$

The Peierls stress,* τ_p, is given by

$$\tau_p = \frac{(\Gamma c-\Gamma o)}{16b^2\alpha} \left(3 + \sqrt{1 + 8\alpha^2}\right) \sqrt{8\alpha^2 - 2 + 2\sqrt{1 + 8\alpha^2}} \tag{5}$$

In the computations, $R = \frac{\Gamma m}{\Gamma o}$ and α were used as independent variables.

Figure 2 shows the variations of $\frac{\tau_p b^2}{\pi(\Gamma c-\Gamma o)}$ with α, and the variations of $\frac{2U_k\pi}{b\Gamma o}$ with α for R = 1.01. The dotted lines for $-1 \leq \alpha \leq 1$ correspond to sinusoidal hills type, Dorn and Rajnak.[2] $\frac{2U_k\pi}{b\Gamma o}$ is closely proportional to $\sqrt{R - 1}$.

Figures 3 and 4 respectively show the variations of $\frac{U_n}{2U_K}$ and $v^* \frac{\tau p}{2U_K}$ (v^* being the activation volume defined by $v^* = -\frac{\partial U_n}{\partial \tau^*}$) as a function of the applied stress τ^*, for some values of α, and R = 1.01. For a given α and ratio τ^*/τ_p, $U_n/2U_K$ and $v^* \frac{\tau_p}{2U_K}$ were found insensitive to physically acceptable ranges in R (i.e. $1.01 \geq R \geq 1.004$).

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*From Fig. 1 a Peierls stress of 53.6 kg/mm^2 is deduced for iron, in good agreement with experimental values, Wynblatt and Dorn.[3]

Curves of Figs. 3 and 4 are broken for $0.1 < \frac{\tau^*}{\tau_p} < 0.3$. In this range of stresses the dislocation can lie in the intermediate valley. The present data refer to the case of a single activation for surmounting the double hump; the plotted activation energy is obtained by adding the two partial activation energies necessary to overcome each hump. Nevertheless the strain-rate, in fact, consists of three terms (one for each partial jump, and one for the previously considered single jump). Because the densities of dislocation lying in the deep and intermediate valleys are different, and likewise the areas swept out and the double kink widths for each partial jump, the formulation of the strain-rate no longer follows the simple form of a single thermally activated process. For these reasons the plots of Figs. 3 and 4 in the range $0.1 < \tau^*/\tau_p < 0.3$ are probably approximate.

As outlined by Guyot and Dorn[4] the curves of Figs. 3 and 4 differ appreciably from the corresponding curves for sinusoidal hills at high stresses. For a Peierls mechanism U_n is proportional to the absolute temperature, and therefore, as shown in Fig. 3, a zero slope stress-temperature is predicted at the absolute zero.

Similar analyses will be done in the future from the knowledge of the potential barriers for screw dislocations and edge dislocations of other orientations in body-centered cubic metals.

REFERENCES

1. R. Chang and L. J. Graham, to be published.
2. J. E. Dorn and S. Rajnak, Trans. AIME, 230, 1052 (1964).
3. P. Guyot and J. E. Dorn, Conference on Deformation of Crystalline Solids, Ottawa (1966), to be published.
4. P. Wynblatt and J. E. Dorn, UCRL-16601 (1965).

ACKNOWLEDGEMENT

This research was conducted as part of the Inorganic Materials Research Division of the Lawrence Radiation Laboratory, Berkeley. The author wishes to express his appreciation to the United States Atomic Energy Commission for their support of this effort. He also thanks Professor John E. Dorn for stimulating discussion.

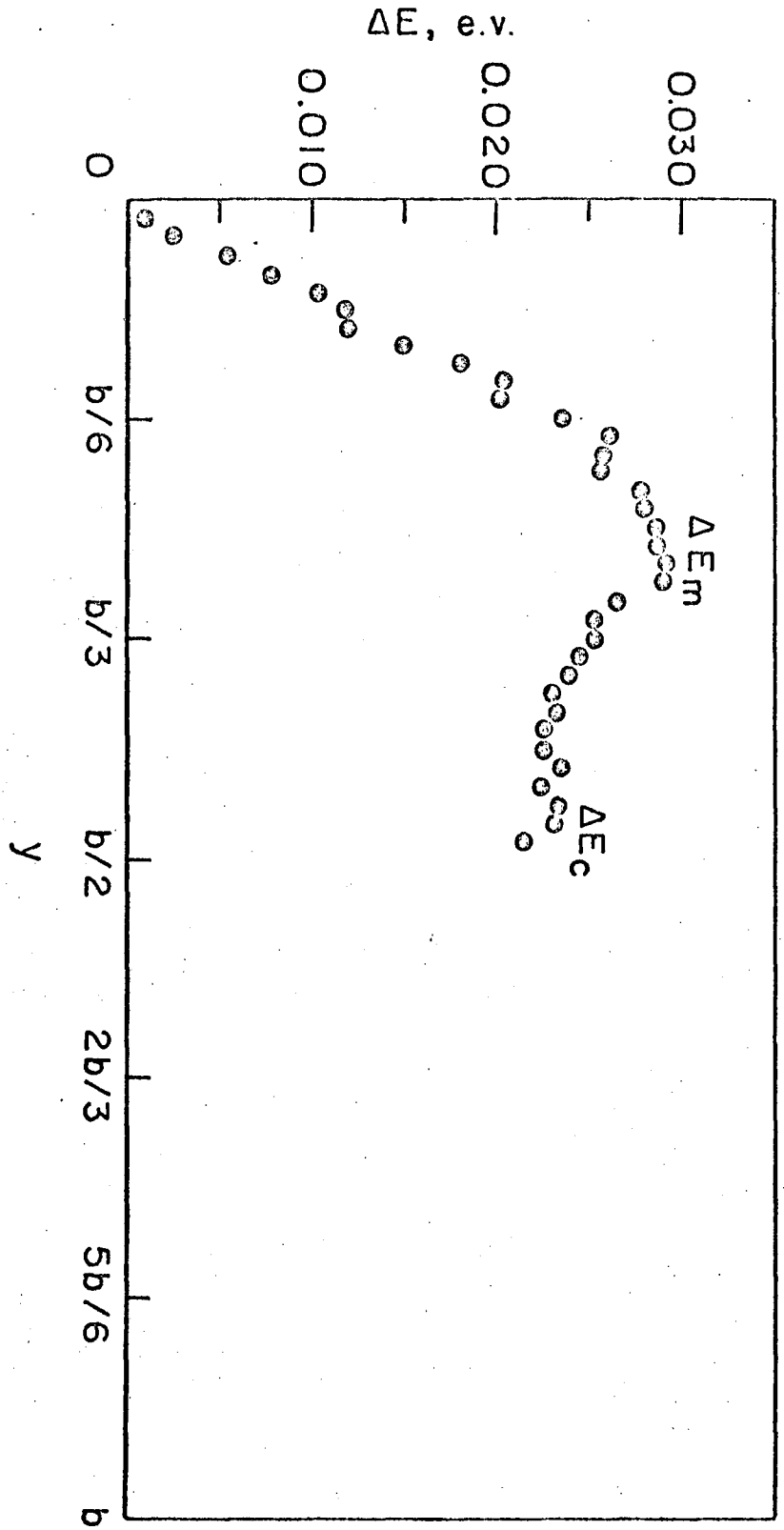

Figure 1. ΔE versus distance moved in the [111] direction

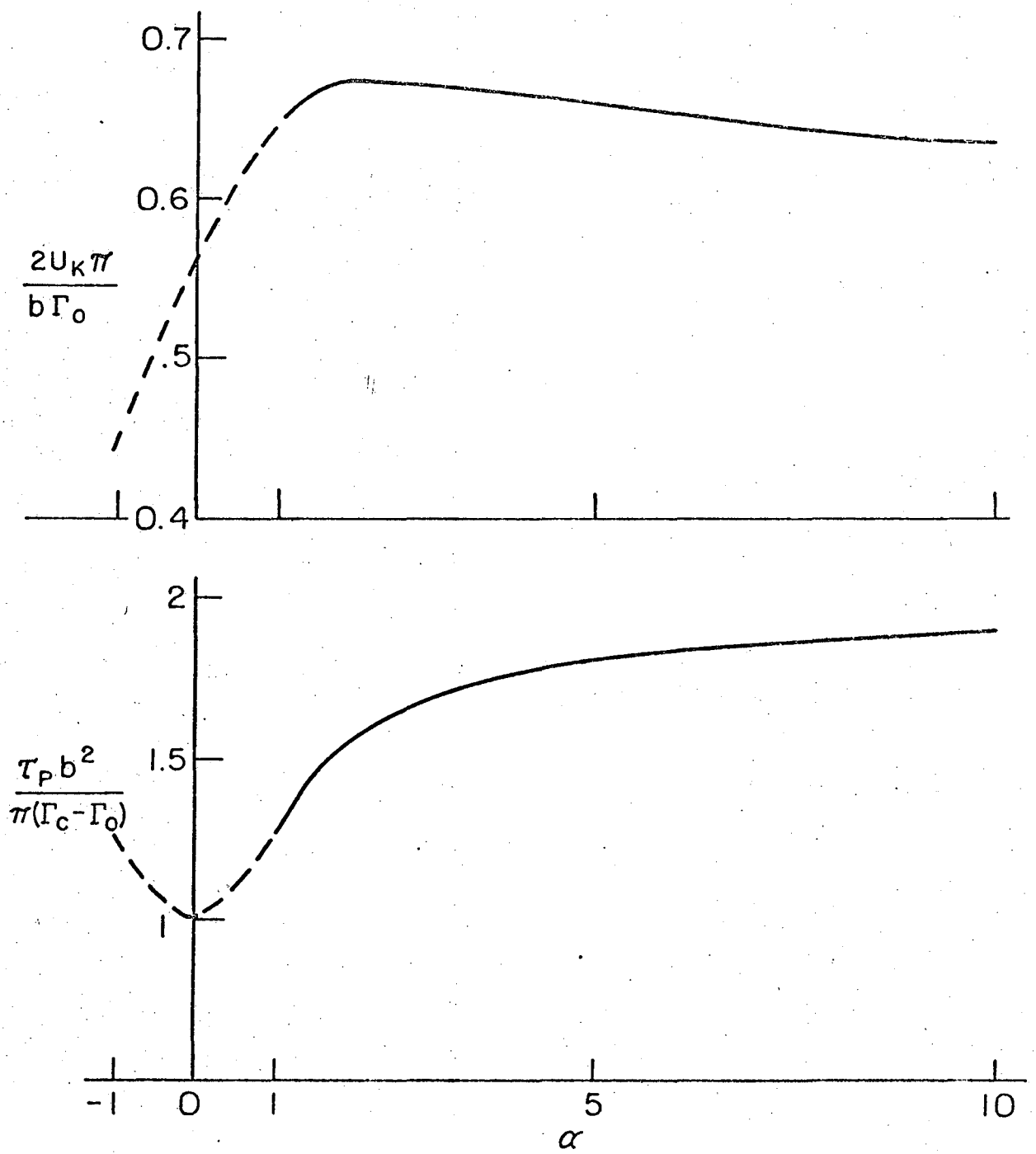

Figure 2. Kink energy and Peierls stress. R = 1.01

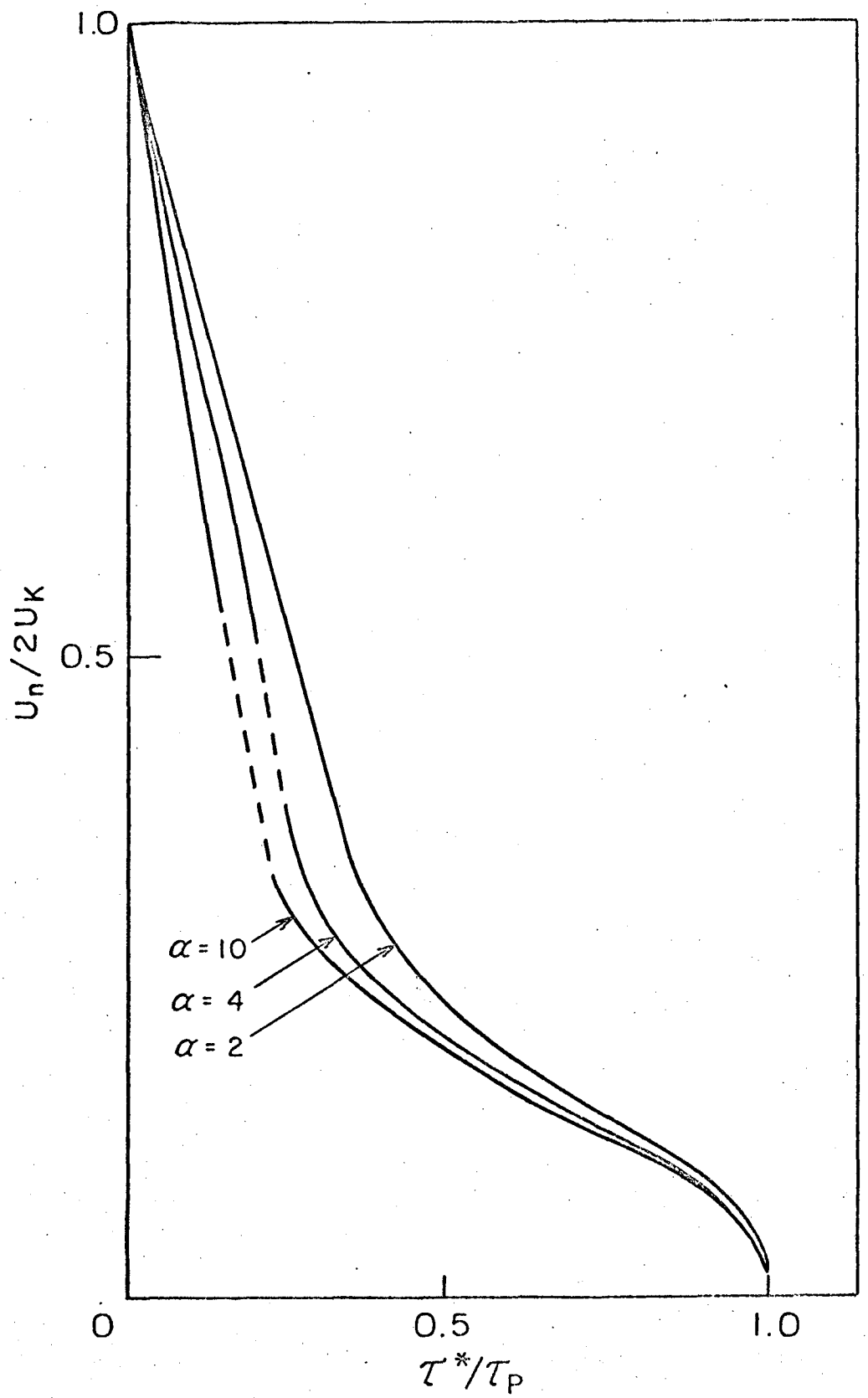

Figure 3. Energy to nucleate a pair of kinks

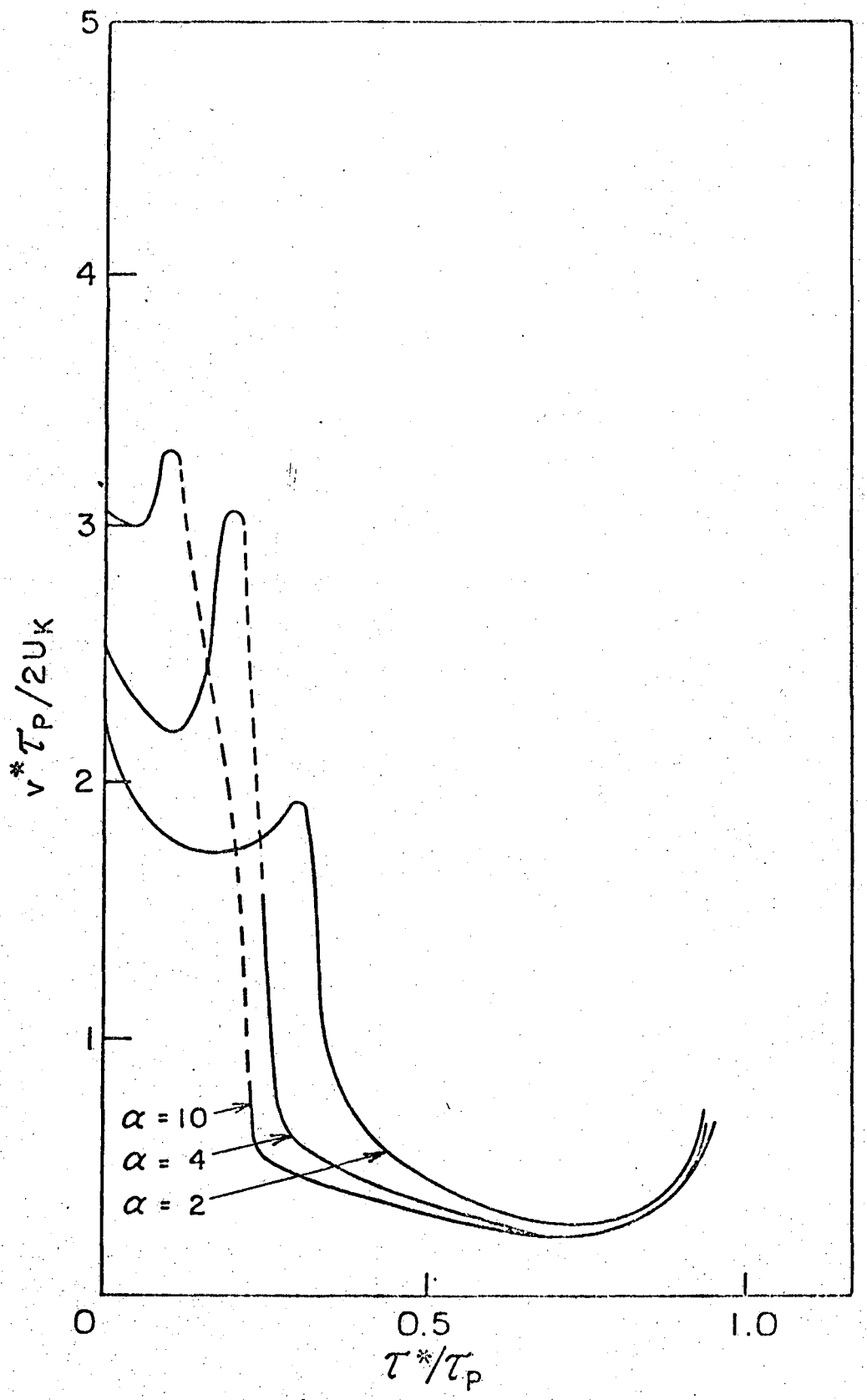

Figure 4. Activation volume

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