FOREWORD

This report was prepared by the Advanced Metallurgical Studies Branch. It was initiated under Project 7353, "Characterization of Solid Phase and Interphase Phenomena in Crystalline Substances," Task No. 735302, "Correlation of Physical and Mechanical Properties of Metals and Ceramics." The work was administered under the direction of the Metals and Ceramics Laboratory, Directorate of Materials and Processes, Aeronautical Systems Division, Deputy Commander/Technology, Wright-Patterson Air Force Base, Ohio. Harold L. Gegel was the project engineer.

This work covers research performed from January 1962 to March 1962.

ABSTRACT

A theoretical investigation was undertaken to determine the stacking fault energy for face-centered cubic metals. An expression was derived which relates the Debye characteristic temperature of the metal and the absolute temperature to the stacking fault energy. An Einstein oscillator was used as a model for the derivation.

This technical documentary report has been reviewed and is approved.

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INTRODUCTION

The formation and occurrence of crystal imperfections known as stacking faults is important to the mechanisms and models postulated to explain work hardening and recovery of close-packed metals and alloys. Stacking faults represent disorders in stacking atomic planes which are formed during the process of crystal growth, plastic deformation, phase transformations, and by the condensation and collapse of vacancy discs. In the face-centered cubic F.C.C. structure the stacking fault is a thin slab of hexagonal close-packed H.C.P. structure, and in H.C.P. material the stacking fault is a thin layer of F.C.C. structure. The faults are formed when disorders in stacking the close-packed layers occur.

F.C.C.	ABCABCABC	⟶	ABCACABCA
	or	⟶	ABCBABCABC
H.C.P.	ABABABAB	⟶	ABABCBCBC
	or	⟶	ABABCACAC
	or	⟶	ABABCABAB

In close-packed lattices it is possible to dissociate a perfect dislocation into a pair of extended dislocations. The degree of extension is determined by the balance between the surface tension of the stacking fault and the elastic repulsion between the partial (half-plane) dislocation. A perfect edge dislocation (1) is dissociated into two partial dislocations according to the relations:

$$\underline{\text{F.C.C.}} \qquad a/2\ [110] = a/6\ [2\bar{1}1] + a/6\ [12\bar{1}]$$

and

$$\underline{\text{H.C.P.}} \qquad a/3\ [11\bar{2}0] = a/3\ [10\bar{1}0] + a/3\ [01\bar{1}0]\ .$$

The equilibrium spacing, d_o, between the partial dislocations is related to the function $\gamma C/Gb^2$, where C is the separation between glide planes, γ is the stacking fault energy, G is the shear modulus, and b is the modulus of the complete Burger's vector. Where the stacking fault energy is low as in gold and lead, the separation of the partial dislocations is large. Conversely, if γ is large, d_o is small. Some experimental values for the stacking fault energies of face-centered cubic metals are presented in table 1 (13) (14).

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TABLE I

STACKING FAULT ENERGIES OF SOME FACE-CENTERED CUBIC METALS

METAL	STACKING FAULT ENERGY (Ergs / Cm^2)
Cu	160, 169
Au	30
Al	238, 230, 170
Ag	43

Seeger (2) (3) has attempted to classify the close-packed metals into groups according to their relative stacking fault energies. Copper, silver, and gold have low stacking fault energies; aluminum, magnesium, zinc, and cadmium have high stacking fault energies. The transition elements nickel, palladium, and platinum fall into a high stacking fault energy category. Later considerations by Seeger (3) suggest that these metals have low stacking fault energies. Nickel (4) has been reported to have either a low stacking fault energy or a high one depending on the way the experimental data is interpreted. An allotropic phase transformation which leads to two different close-packed structures may be responsible for the high and low values of γ experimentally determined (5) (6).

Seeger has suggested that the reason for this difference in stacking fault energy between these two groups of metals is that the Brillouin zones of the monovalent metals are only half full and therefore the electrons at the Fermi level do not strongly interact with the Brillouin surface. In contrast, the Brillouin zones of the polyvalent metals are filled with some overlap into the next zone. The overlaps cause a strong interaction of the Fermi surface with the Brillouin surface.

Since there are apparent discrepancies in the classification of the metals into groups having high and low stacking fault energies according to their valency characteristics, a better more general method for estimating γ is needed. We use a semiempirical approach to derive a method for estimating γ for face-centered cubic metals.

DISCUSSION

Stacking Fault Energy Equation

The expression deduced in this report is based on a relationship between experimentally determined stacking fault energies of some face-centered cubic metals and the average atomic weight of the atom. When logarithm of the stacking fault energy is plotted as a function of the average atomic weight M a straight line can be drawn through the points.

This relationship is plotted in figure 1. Since γ is a function of the mass of an atom, it is reasonable to assume that the stacking fault energy is fundamentally related to the nature of lattice vibrations. The equation for the line plotted in figure 1 is

$$\gamma = \gamma_0 \exp(-SBM) \tag{1}$$

where γ_0 is the extrapolated value at zero atomic weight, SB is the slope, and M is the average atomic weight of the metal. It is assumed that the slope consists of two terms. The product SB will have the dimensions of energy/mass. S consists primarily of the energy of a displaced atom from its equilibrium position, and B is an undetermined multiplier which gives SB the correct dimensions. The first derivative of equation (1) is

$$d\gamma/dM = SB \exp(-SBM) \tag{2}$$

The dimensions of the left-hand side of equation (2) are energy/mass; the dimensions on the right-hand side must subsequently be equal to the left-hand side. If the usual assumption governing the potential energy of the motion of the atoms is made, i.e., the interaction energy of the atom with its surrounding is nearly harmonic and is a function of its relative displacement to its neighbor's a relationship for γ can be deduced that will explain the curve presented in figure 1. Considering the crystal to be an Einstein type solid, we can write for the potential energy

$$E = 1/2\ k_s \overline{x}^2 \tag{3}$$

where k_s is the lattice force constant and $\overline{x}^2$ is the mean square displacement of the atoms from their equilibrium positions. k_s is related to the vibration frequency by

$$k_s = (2\pi\nu)^2 / M \tag{4}$$

The mean square displacement of the atoms $\overline{x}^2$ for an Einstein oscillator is

$$\overline{x}^2 = 3h^2 T / (2\pi)^2\ Mk\theta^2 \tag{5}$$

Substituting equations (4) and (5) into equation (3), we obtain for the potential energy

$$E = 3/2\ h\nu\ T/M^2\theta \tag{6}$$

It is interesting that the stacking fault energy is a function of temperature which is introduced by the dependence of the potential energy E of the lattice on the absolute temperature T. B must have the dimensions of mass/energy, if the exponent SBM is to be dimensionless. Assuming that B has the relationship

$$B = M/h\nu \tag{7}$$

we can write for the slope SB

$$SB = 3/2\ (T/\theta)/M \tag{8}$$

Substituting equation (8) into equation (1), the expression for γ becomes

$$\gamma = \gamma_0 \exp(-3/2\, T/\theta) \qquad (9)$$

The relationship between γ and M may be strictly fortuitous, since the expression deduced to explain the curve presented in figure 1 shows γ to be a function of (T/θ). Log γ as a function of T/θ is plotted in figure 2. The data presented in table 1 must therefore represent an average temperature between ambient and absolute zero. The technique used by Seeger and Berner depended upon the determination of τ_{III}, the shear stress at the start of stage III deformation for face-centered cubic metals, as a function of temperature. This experimental technique for the determination of stacking fault energy does not give a stacking fault energy-temperature relationship. The functional relationship between γ and (T/θ) is a reasonable one, since it compares all metals at the same amplitude of vibration.

Classification of Face-Centered Cubic Metals

Equation (9) is used to devise a classification system for face-centered cubic metals. Calculated values of $\log\gamma$ are plotted against the absolute temperature T. According to the groups of metals plotted in figure 3, the metals can be placed into three groups based on their relative stacking fault energy. Lead, thorium, gold, strontium, silver, and platinum are metals having low stacking fault energies. Palladium, iridium, and copper have intermediate stacking fault energies, and aluminum and nickel have high stacking fault energies. It is apparent that many of the metals in the low stacking fault energy group are polyvalent and one is a transition metal. Transition metals fall into all three classifications. It is evident that metals can not be separated into groups according to their valency without knowing in considerable detail about their bonding and electronic structure. The positions of aluminum, nickel, and copper are in agreement with those established by Hardwick and Tegart (7) who investigated structural changes in these metals during hot torsion deformation. The structural changes that occurred in these metals were dependent on the rates of climb of dislocations. The rates of climb of dislocations in metals having a high stacking fault energy will be greater than those which have a low stacking fault energy. The structure of aluminum showed only polygonization; the structure of nickel showed a combination of recrystallization and polygonization, and copper showed only recrystallization. Since polygonization requires dislocation climb to occur, the order of decreasing stacking fault energy is aluminum, nickel, and copper.

Calculation of Stacking Fault Energies for Some Hexagonal Close-Packed and Body Centered Cubic Metals

Stacking fault energies for several hexagonal close-packed and body centered cubic metals were calculated using the derived equation. These results are presented in table 2. The position of each metal according to its relative order of magnitude agrees closely with the Seeger classification. Cadmium is an exception. Seeger's original classification considered it to have a high stacking fault energy; this system predicts that cadmium has a low stacking fault energy.

TABLE 2

CALCULATED STACKING FAULT ENERGIES FOR SOME HEXAGONAL CLOSE-PACKED AND BODY CENTERED CUBIC METALS

METAL	-ergs/cm^2-300°K	-ergs/cm^2-500°K	-ergs/cm^2-100°K
Mg	52	18.5	145
Be	155	115	210
Zn	55	20	150
Zr	37	10.5	130
Cd	18	3.0	108
Nb	55	20	150
Mo	74	34	165
Fe	84	40	170

Some investigators have attempted to determine the frequency of faulting in cold-worked structures by determining stacking fault probabilities through x-ray diffraction techniques. Metals having a high stacking fault probability will have a low stacking fault energy by this theory, and, similarly, metals with high stacking fault energies have low stacking fault probabilities.

Stacking Fault Probability Considerations

Wagner (8) (9), Taranto and Brotzen, (10) McHargue, (11) and Smallman and Westmacott (12) have determined stacking fault probabilities for aluminum, nickel, copper, silver, cerium, and thorium which were plastically deformed at liquid oxygen and room temperatures. The results of these investigators are presented in table 3.

TABLE 3

STACKING FAULT PROBABILITIES AND RECIPROCAL STACKING FAULT PROBABILITIES

METAL	TEMP	STACKING FAULT PROB. α	α^{-1}	REF.
Ni	LIQ. OXYGEN	0.005 - 0.006	200-167	(9)
Cu	LIQ. OXYGEN	0.012	83	(10) (13)
Ag	LIQ. OXYGEN	0.017	59	(12)
Al	LIQ. OXYGEN	0.003	333	(12)
Ce	ROOM TEMP.	0.018	55	(12)
Th	ROOM TEMP.	0.019	53	(12)

The values of the various stacking fault probabilities indicate that the value of stacking fault energy for each metal arranged in order of decreasing magnitude is aluminum, nickel, copper, silver, cerium, and thorium. This arrangement is in good agreement with the calculated positions. The reciprocal of the stacking fault probability is an indication of the spacing of the faults between the close-packed planes. In the case of aluminum, a fault occurs for each 333 planes of close packed metal. Because the material is not in equilibrium, the best to expect from stacking fault probability determinations is an order of magnitude estimate of the stacking fault energy.

When the stacking fault probabilities are compared to the calculated stacking fault energies for the temperatures at which they were deformed, it becomes apparent that the magnitude of the stacking fault energy cannot be determined accurately from a knowledge of the stacking fault probability. A plot of the stacking fault probability α as a function of the stacking fault energy γ is made in figure 4. This plot shows that α reaches a plateau when γ is = 100 ergs/cm^2 for face-centered cubic structures. When α is equal to about 0.018 γ can vary between $0<\gamma\leq 100$ ergs/cm^2. For values of $\gamma>100$ ergs/cm^2 a more reliable estimate of the stacking fault energy can be made from a knowledge of the stacking fault probability.

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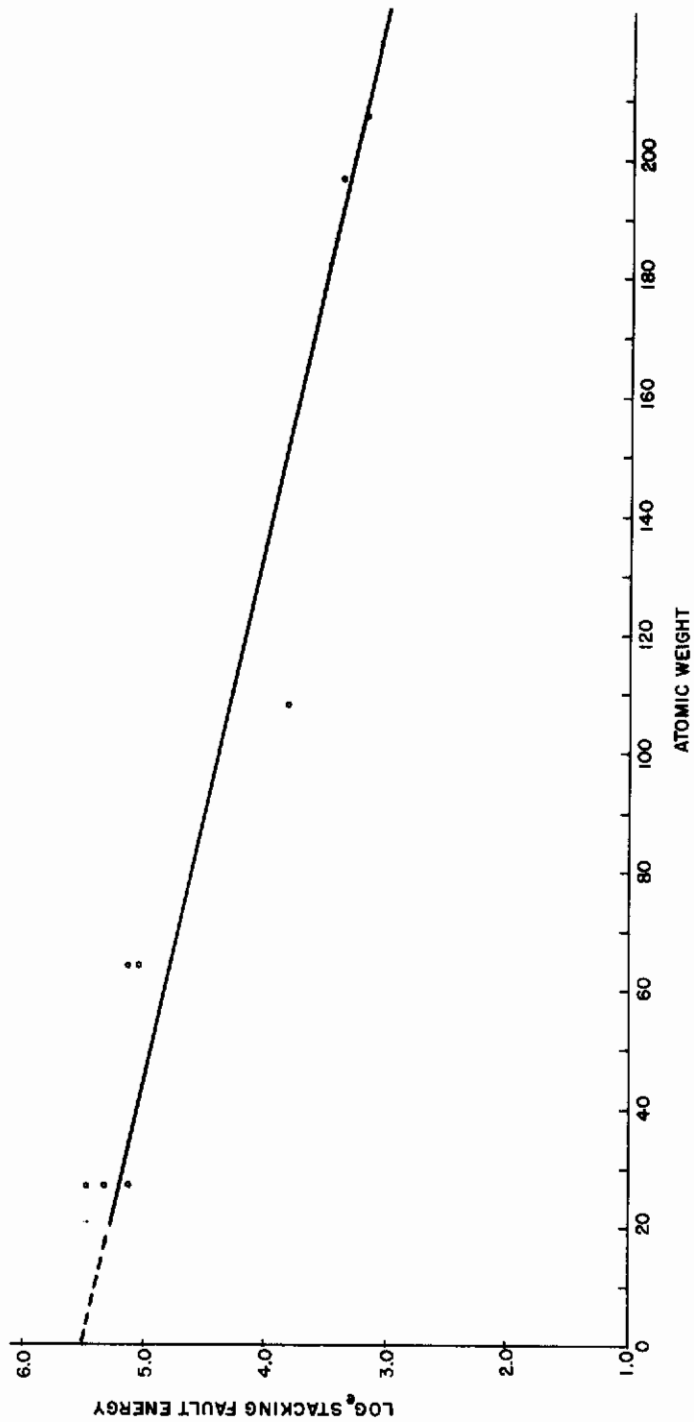

Figure 1. Log$_e$ Stacking Fault Energy of Face-Centered Cubic Metals As a Function Of Their Atomic Weights

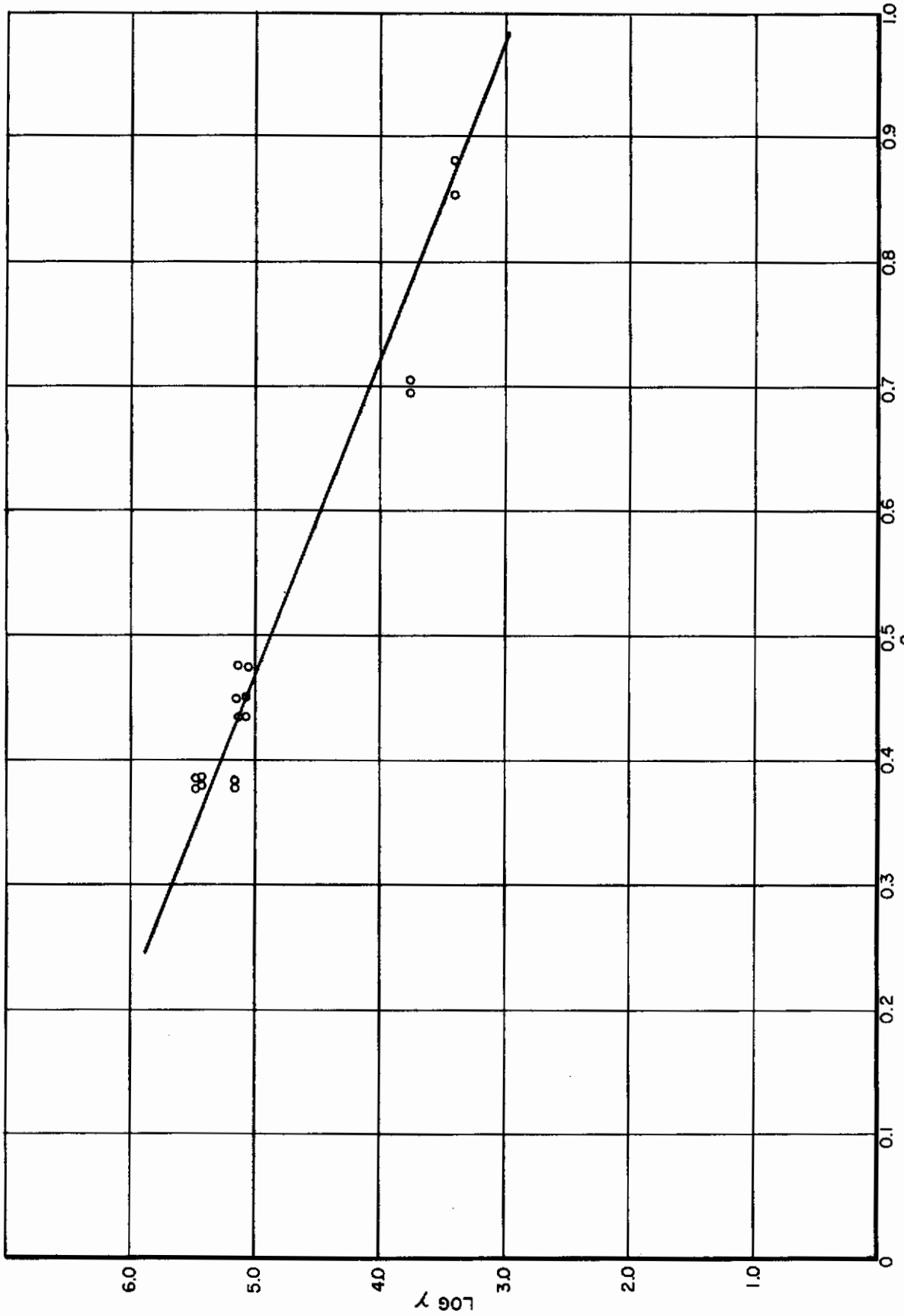

Figure 2. Log γ As a Function of T/θ

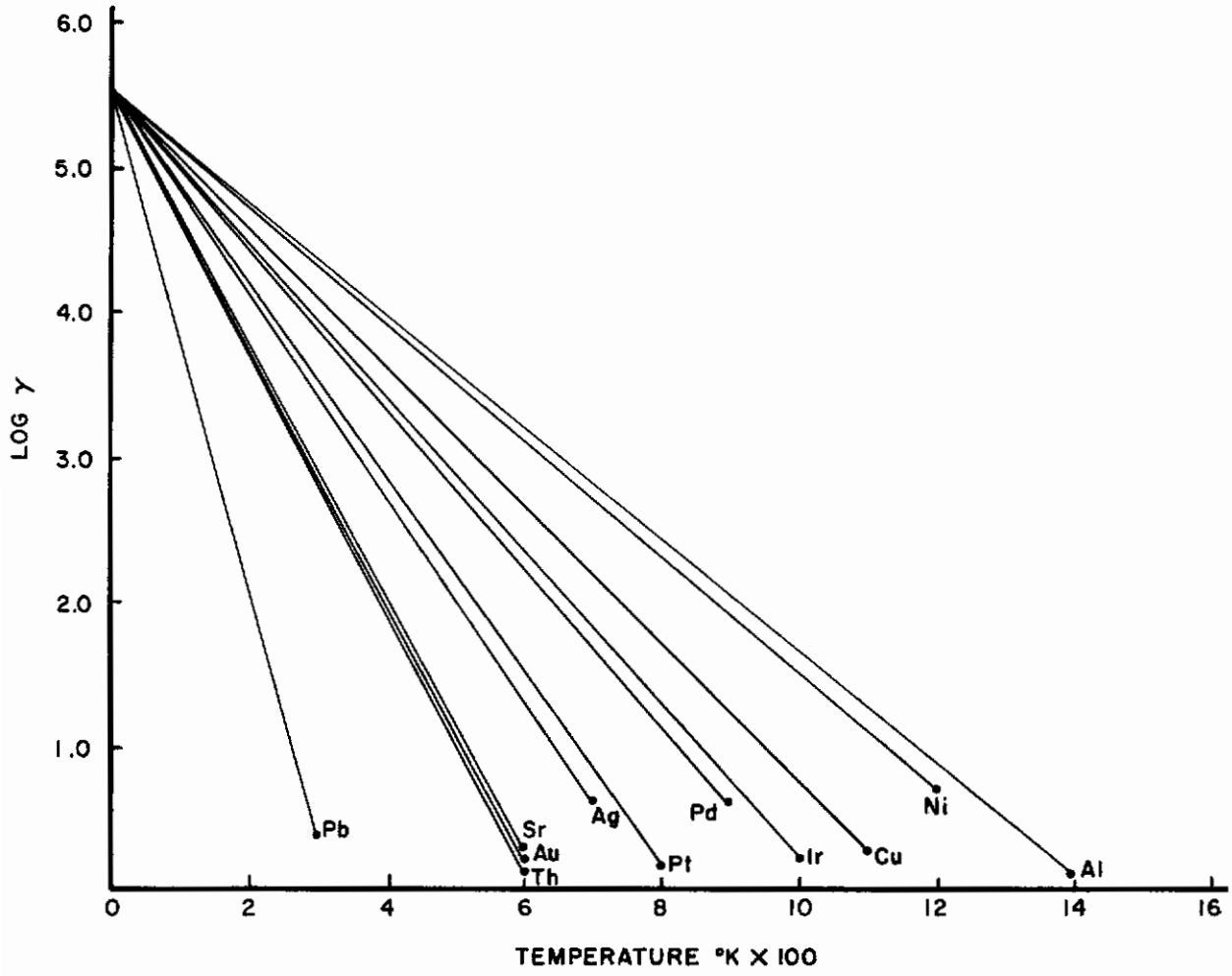

Figure 3. Stacking Fault Energies for Face-Centered Cubic Metals as a Function of Temperature

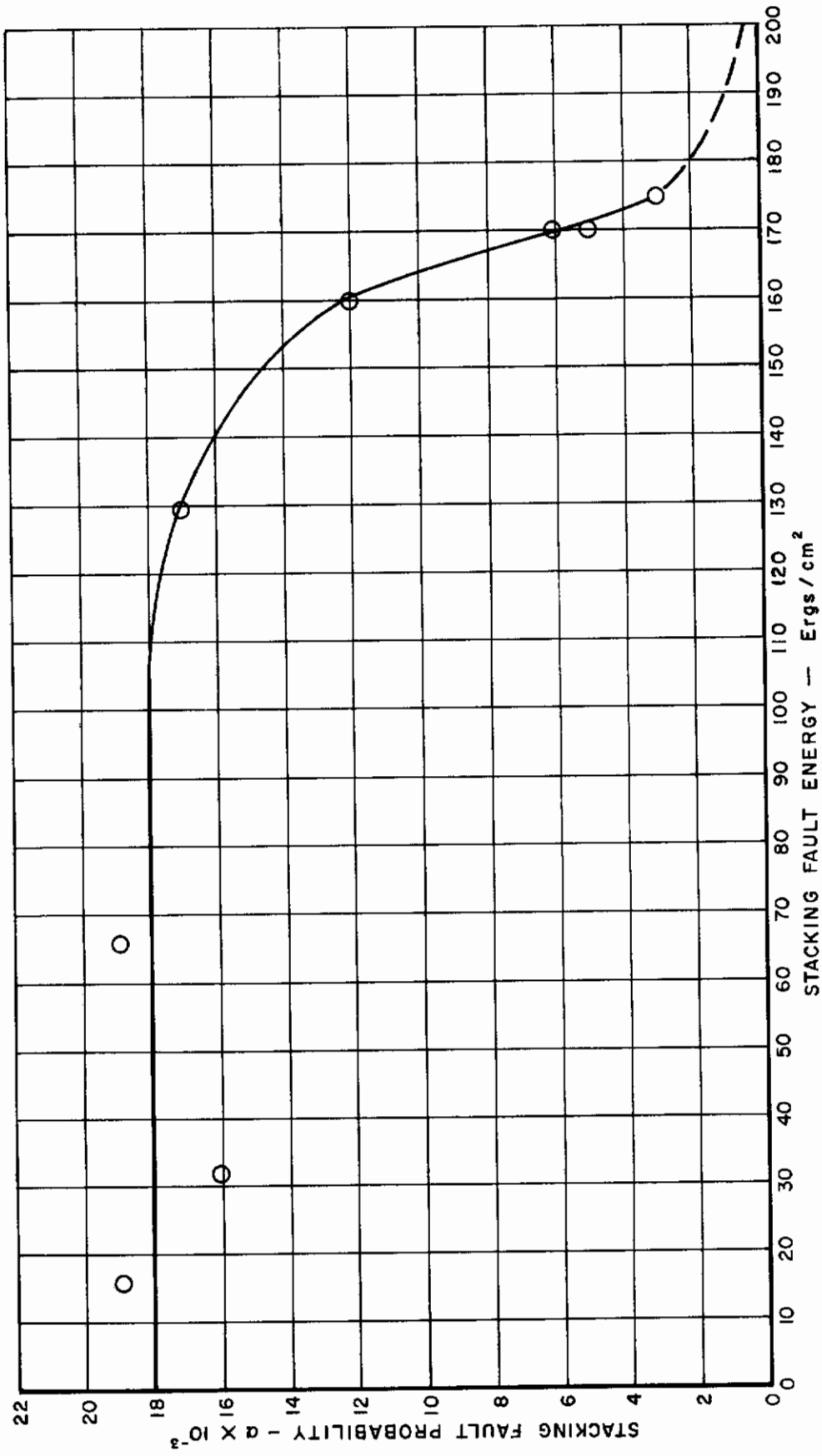

Figure 4. Stacking Fault Probability α As a Function of the Stacking Fault Energy γ