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A NEW METHOD FOR DETERMINATION OF STACKING FAULT ENERGY OF PURE METALS BY X-RAY DIFFRACTION

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Dedicated to the memory of Late Professor S. P. Sen Gupta
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An indirect method for the determination of stacking fault energies (SFE) of pure metals by X-ray diffraction technique is reported. The existing methods for the calculation of SFE suffer from simplified assumptions regarding dislocation distribution and type of dislocation present in the specimen. The present method is based on the strain field model of dislocations assuming a restrictedly random dislocation distribution. The method is applied for the calculation of SFE of plastically deformed copper and the values come out to be very close to those obtained from direct observation methods like TEM.

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1. Introduction

The stacking fault energy (SFE) of close packed metals influences their physical properties. All mechanical phenomena, which are related to dislocation motion and the resulting dislocation configurations, are a strong function of the separation of partial dislocations, which is determined by the SFE. From the measurement of geometry of some dislocation configuration [1 − 2] SFE can be measured directly provided the stacking fault energy is relatively low, typically less than 30 mJ/m^2 for extended modes. The weak-beam method of electron microscopy allows dislocations to be imaged as two relatively intense lines if they are separated by a distance of

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more than 20 Å. The stacking fault energy is directly related to the separation of Schokley partials [3]. From the analysis of the weak beam images of dissociated dislocations in copper, γ_{Cu} has been found to be (41 ± 9) mJ/m^2 [3–5].

Among the indirect methods of measurement, deformation stacking fault probability (α) and dislocation density (ρ), simultaneously from X-ray diffraction studies, also leads to the determination of stacking fault energy of deformed alloys, and a proper extrapolation may lead to the determination of SFE of pure metals. In the present work, the existing method of determination of SFE is reviewed. A new method has been proposed which takes into account the dislocation types and distributions which eventually helps in determining SFE of pure metals.

2. *Theoretical formulation*

The stacking fault energy is expressed as

$$\gamma = G(\boldsymbol{b}_2 \cdot \boldsymbol{b}_3)/(2\pi\eta r)\,, \tag{1}$$

where G is the shear modulus and can be calculated from the elastic constants c_{ij}, $\boldsymbol{b}_2$ and $\boldsymbol{b}_3$ are Burgers vector for the partial dislocations, η is the type of dislocation and r is width of intrinsic stacking fault ribbon. Further, the deformation stacking fault probability (α) is defined as

$$\alpha = \rho r d\,, \tag{2}$$

where d is the interplanar spacing of the slip plane. For a F.C.C system, the stacking fault energy can be written as [6].

$$\gamma = Ga^3\rho/(\alpha\eta 24\pi\sqrt{3})\,. \tag{3}$$

This simple equation can be used to evaluate the stacking fault energy γ provided the type of dislocation (η) is known, while α and ρ are measured from X-ray diffraction line profile analysis. The value of η changes from $\eta = 1$ (for screw dislocation) to $\eta = (1 - n)$ (for edge dislocation), where 'n' is the Poisson's ratio. Thus the uncertainty remains if η is not known a priori. A further limitation of Eq. (3) is that the dislocation density ρ and stacking fault probability α should be measured simultaneously, which often involves simplified assumption regarding dislocation distribution. Further, X-ray diffraction line profile analysis based on the breadth of X-ray diffraction lines give the value of formal dislocation density ρ^*. For a random dislocation distribution, ρ^* is related to the mean square strain $\langle\epsilon_L^2\rangle$ by the Williamson Smallman equation

$$\rho^* = K\langle\epsilon_{50}^2\rangle/b^2,$$

where $\langle\epsilon_{50}^2\rangle$ is the mean-square strain at a coherence length of 50 Å. The formal dislocation density ρ^* is related to the true dislocation density ρ by the relation

$\bar{C}_{hkl}\rho^* = \rho$ where $\bar{C}_{hkl}$ is the contrast factor expressing the visibility of dislocation in any diffraction experiment. In all previous work the value of $\bar{C}_{hkl}$ was chosen to be 1 which results in systematically lower values of γ. Further, if the dislocation distribution differs from a random one, the determination of ρ becomes erroneous. The constant K depends on the crystal geometry, nature of strain distribution and shape of strain broadened profile.

The equation of Smallman and Westmacott can be modified by incorporating the dislocation contrast factor $\bar{C}_{hkl}$, so the equation reduces to

$$\gamma = Ga^3 C_{hkl}\rho^*/(\alpha\eta 24\pi\sqrt{3})\,. \tag{4}$$

Reed and Schramm [7] have modified Eq. (3) as

$$\gamma = \frac{A_i^{-0.37} K_{111}\omega_0 G_{111} a_0 \langle\epsilon_{50}^2\rangle_{111}}{\pi\sqrt{3}\,\alpha}\,, \tag{5}$$

where the uncertainty due to η is absorbed in the constant factor $K_{111}\omega_0$. A_i is the anisotropy factor defined as $A_i = 2C_{44}/(C_{11} - C_{12})$ and C_{ij} are elastic stiffness constants. However, if the dislocation type and arrangement changes with alloying, which is often the case, a constant value of $K_{111}\omega_0$ is not a reasonable assumption. The value of $K_{111}\omega_0$ was obtained as 6.6 by Reed and Schramm.

Further, the mean square strain is a strong function of coherence length L and dislocation distribution. For dislocation-induced strain broadening, $\langle\epsilon_L^2\rangle$ is expressed as either

$$\langle\epsilon_L^2\rangle = \rho\bar{C}_{hkl}(b^2/4\pi)f(\chi), \qquad \chi = (1/2)\exp(-0.25)\exp(2R_e/L)$$

(The expression for $f(\chi)$ can be found elsewhere [8]),
or

$$\langle\epsilon_L^2\rangle = \rho\bar{C}_{hkl}(b^2/4\pi)\ln(R_e/L)$$

in a simplified manner for a weak defect correlation. $\bar{C}_{hkl}$ is the contrast factor corresponding to the indices hkl and is defined as $\bar{C}_{hkl} = C_{100}(1 - qH^2)$ with $H^2 = 1/3$ for the index 100.

The stacking-fault energy can be obtained by modifying the expression given by Reed and Schramm [7, 9]. Incorporating the strain field model of dislocations the expression for SFE reduces to either

$$\gamma = \frac{A_i^{-0.37} K_{111}\omega_0 G_{111} a_0}{\pi\sqrt{3}\,\alpha}\left\{(b/2\pi)^2(\pi\rho\bar{C}_{111})f(\chi)\right\}, \tag{6}$$

or using approximate strain function it becomes,

$$\gamma = \frac{A_i^{-0.37} K_{111}\omega_0 G_{111} a_0}{\pi\sqrt{3}\,\alpha}\left\{(b/2\pi)^2(\pi\rho\bar{C}_{111})\ln(R_e/L)\right\}. \tag{7}$$

3. Results and discussion

Stacking fault energy of pure copper has been determined by using the formalism described in the earlier section. The cold-worked copper powder has been prepared by filing at room temperature [10]. Microstructural characterization has been done using a model based approach. A restrictedly random dislocation distribution and log-normal distribution of spherical crystallites was used as the microstructural model. The method of analysis and corresponding results can be found elsewhere [10]. Only the results which are relevant for the analysis of stacking fault energy are given in Table 1.

TABLE. 1. Microstructural parameters and some physical constants of Cu.

ρ ($10^{15} m^{-2}$)	$\bar{C}_{111}$	α	G_{111} (10^{11} Pa)	a_0 (nm)	R_e (nm)	q
10.2 ±0.02	0.067	0.003	0.405	0.3614 ±0.00017	7.4 ±1.1	2.34 ±0.02

TABLE. 2. Value of γ determined from different equations.

From equation (4)	58.6 $\mathrm{mJm^{-2}}$
From equation (8)	16.7 $\mathrm{mJm^{-2}}$
From equation (9) ($R_e = L/2$)	9.5 $\mathrm{mJm^{-2}}$
From equation (10) ($\chi = 1$)	25.7 $\mathrm{mJm^{-2}}$
From equation (11)	14.5 $\mathrm{mJm^{-2}}$

The stacking fault energies have been calculated from the expressions (6) and (7) and are shown in Table 2. It is clear from the nature of expression (5) that γ is a function of χ, which is further related to the averaging length inside the crystal. Reed and Schramm used an L value of 5 nm to calculate stacking fault energy. However, it is reasonable to calculate the stacking fault energy within a sub area of radius R_e characterizing the dislocation substructure. In the present case, it is assumed that if $\chi = 1$, which corresponds to $2.877L = R_e$, provides a value of $L \sim 2.5$ nm. The stacking fault energy is calculated from Eq. (6) using $\chi = 1$. Substituting the value of variables in Eqs. (6) and (7) the stacking fault energy is given by

$$\text{From equation (6)} \qquad \gamma = 13.7 f(\chi)\ \mathrm{mJm^{-2}} \tag{8}$$

$$\text{From equation (7)} \qquad \gamma = 13.7 \ln(R_e/L)\ \mathrm{mJm^{-2}}\,. \tag{9}$$

If the anisotropy correction factor $A^{-0.37}$ is omitted (since the anisotropic factor is also included in the average dislocation contrast factor $\bar{C}_{111}$), the above expressions are modified to

$$\gamma = 21 f(\chi)\ \mathrm{mJm^{-2}}\,, \tag{10}$$

$$\gamma = 21 \ln(R_e/L) \text{ mJm}^{-2} \,. \tag{11}$$

It is clear that from the above Eqs. (7−9) if $L = R_e/2$ ($L = R_e$ does not provide an acceptable value of γ), systematically lower value of γ are obtained.

Table 2 contains also the value of the stacking-fault energy calculated from Eq. (4). The uncertainty of Eq. (3) is the value η, which depends on the type of dislocations. For pure-edge and screw dislocations, the value of γ comes out to be 85 mJm^{-2} and 50 mJm^{-2}, respectively. In cold worked copper sample, the type of dislocations present is governed by the factor q (Table 1). The value of q is 2.34, which is equivalent to 75% screw and 25% edge-type dislocations. Assuming the value of η to be linearly dependent on the type of dislocation, the value of γ is found to be 58 mJm^{-2}. It is worth comparing the results obtained in the present investigation with other experimentally observed values. Table 3 lists the range of γ values. The experimental values are obtained from an extrapolation of those obtained for cold-worked alloys. To estimate SFE of copper and those of the copper alloys with $e/a \geq 1.10$, extrapolation from the values which could be measured (i.e. of alloys with large e/a) were used by several workers and two methods of extrapolation have been suggested: in the first a monotonically rising curve with decreasing e/a is assumed by Howie and Swann [11] which can lead to the value for γ_{Cu} of the order of 70 mJ/m^2 [12]. In the second case, based on the extrapolation methods of Gallagher [13] and Liu and Gallagher [14], using the experimental results of Nordstrom and Barret, the stacking fault energy γ_{Cu} was found to be 50 mJ/m^2 [12].

TABLE. 3. Literature values of γ.

γ (mJm^{-2})	Method
18	Theoretical (tight binding) [15]
45	Experimental [16]
55	Experimental [13]
62	Experimental [6]

It is clear from Table 3 that a reasonably good agreement can be observed for the simplest modified Smallman-Westmacott Eq. (4), provided the true dislocation density and the dislocation type factor can be determined from microstructural modeling.

The value of γ obtained from Eqs. (8)−(11) (modified Reed-Schramm equation) are reasonably close to the theoretical value of γ obtained from tight-binding approach.

4. Conclusion

A new method has been developed by modifying the existing Reed-Schramm method and Smallman-Westmacott method for the determination of stacking fault energy γ for pure metals and alloys. It is clear that microstructural modeling plays a vital role in the determination of γ and it is established from the value of Cu. In the present communication, the results are obtained from the measurement of dislocation density and stacking fault probability on cold-worked metallic copper.

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NOVA METODA ZA ODREĐIVANJE ENERGIJE GREŠAKA SLAGANJA U ČISTIM METALIMA PRIMJENOM RENTGENSKE DIFRAKCIJE

Izvješćujemo o novoj metodi za određivanje energije grešaka slaganja (SFE) u čistim metalima primjenom rentgenske difrakcije. Dosadašnje metode za izračunavanje SFE trpe zbog jednostavnih pretpostavki o raspodjeli i vrsti dislokacija u uzorku. Nova metoda se zasniva na modelu polja naprezanja dislokacija, pretpostavljajući ograničivajuću slučajnu raspodjelu dislokacija. Metodu primjenjujemo za izračunavanje SFE plastično deformiranog bakra i ishodi su vrlo blizi onima koji su postignuti izravnim metodama mjerenja, kao što je TEM.