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EVALUATION OF STACKING FAULT ENERGIES IN FUNCTION OF PRESSURE IN COBALT POWDER

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Previous measurements of stacking fault probabilities (SFP) and root mean square strains (RMSS) were used now to evaluate the stacking fault energies (SFE) in metastable cobalt powder at different external pressures up to 660 MPa. SFE in HCP cobalt increase with growing pressure, while in FCC cobalt there exists a maximum at about 100 MPa, and at higher pressures SFE decrease.

1. Introduction

Stacking faults are an important microstructural component in terms of room-temperature mechanical behaviour of materials, because they may contribute to strengthening and may be structural precursors of twins[1]. Systems which exhibit a very low stracking fault energy, i. e. the energy per unit area necessary to produce a stacking fault, are widely used in biomedical applications, because stacking fault intersections and twins are the main contributors to work hardening behaviour[2]. In addition the SFE affect susceptibility to stress corrosion cracking and electrical resistivity[3].

In this work we discuss the dependence of SFE on pressure at room temperature in FCC and HCP metastable cobalt green compacts, obtained by compaction

of reduced cobalt oxide powder. Previously, the SFP and RMSS in pressed cobalt powder were measured by analysing X-ray diffraction profiles[4], and we now used these data to calculate the SFE in the same samples.

2. Calculation of SFE

Reed and Schramm[5] showed that there exists a linear relationship between SFE and RMSS/SFP ratio and that the SFE for FCC crystals can be expressed as

$$\gamma = \frac{K_{111}\,\omega_0\,G_{(111)}\,a}{12\,\pi\sqrt{3}}\,\frac{\langle\varepsilon_5^2\rangle_{111}}{\alpha}, \tag{1}$$

where γ is stacking fault energy, $G_{(111)}$ is the shear modulus in the (111) fault plane, a is the cubic lattice constant, $\langle\varepsilon_5^2\rangle_{111}^{1/2}$ is root mean square strain in the $\langle 111\rangle$ direction averaged over a distance of 5 nm, α is stacking fault probability for FCC crystals, and K_{111} and ω_0 are constants.

Similarly in hexagonal crystals, where the common slip system is on the basal plane in the closed-packed direction (0001) $\langle 11\bar{2}0\rangle$, the SFE can be expressed as

$$\gamma = \frac{K_{0001}\,\omega_1\,G_{(0001)}\,c}{24\,\pi}\,\frac{\langle\varepsilon_5^2\rangle_{11\bar{2}0}}{\alpha}, \tag{2}$$

where c is the parameter of the hexagonal unit cell, $G_{(0001)}$ is the shear modulus in the (0001) fault plane, $\langle\varepsilon_5^2\rangle_{11\bar{2}0}^{1/2}$ is the root mean square strain in the $11\bar{2}0$ direction averaged over a distance of 5 nm, and α is the stacking fault probability for HCP crystals. Eq. (1) can be rearranged in the form

$$\frac{\gamma}{G_{(111)}\,a} = \frac{K_{111}\,\omega_0}{12\,\pi\sqrt{3}}\,\frac{\langle\varepsilon_5^2\rangle_{111}}{\alpha}, \tag{3}$$

and Eq. (2) in the form:

$$\frac{\gamma}{G_{(0001)}\,c} = \frac{K_{0001}\,\omega_1}{24\,\pi}\,\frac{\langle\varepsilon_5^2\rangle_{11\bar{2}0}}{\alpha}, \tag{4}$$

In order to determine the SFE for FCC cobalt we used the method of calculation and the data for elements Ag, Au, Cu and Ni given by Reed and Schramm[5]. To determine the constant $K_{0001}\omega_1$ in Eq. (4) we used data from the available literature for SFE, RMSS and SFP of hexagonal metals Ti, Co and Mg. Relevant data for these elements are presented in Table 1.

SFE complied from literature and given in Table 1, are plotted versus $\frac{\langle\varepsilon_5^2\rangle}{\alpha}$ data in Fig. 1. The slope of the line in Fig. 1 is $K_{0001}\omega_1/24\Pi$ and from this constant, using Eq. 2, we could calculate the SFE for pressed hexagonal cobalt powder.

TABLE 1.

ELEMENT	γ/mJm^{-2}	Ref.	$a \cdot 10^3$	$\langle \varepsilon_5^2 \rangle_{11\bar{2}0}^{1/2} \cdot 10^3$	Ref.	$G_{(0001)} \cdot 10^{-11}$/Pa	Ref.	$c \cdot 10^{10}$/m	$\frac{\gamma}{G_{(0001)} c} \cdot 10^4$	$\frac{\langle \varepsilon_5^2 \rangle_{11\bar{2}0}}{a} \cdot 10^4$	$\frac{K_{0001}\omega_1}{24\pi}$	$K_{0001}\omega_1$
Ti	12.2	9	8.8 ± 0.6	1.6 ± 0.5	9	0.467	6	4.68815	5.57	3.06	1.82	137.2
Mg	24.7	9	0.69 ± 0.06	0.75 ± 0.06	9	0.1658	7	5.210698	28.59	8.86	3.23	243.5
Co	31.0	3	24.3 ± 7	3.0 ± 0.1	4	0.755	8	4.06890	10.09	3.79	2.66	200.7

Experimental data used in Eq. (2).

TABLE 2.

Metal	$A = \frac{2C_{44}}{C_{11} - C_{12}}$	Reference	$K_{0001}\omega_1$	$A^{-1.9}$	$\frac{\langle \varepsilon_5^2 \rangle_{11\bar{2}0}}{a} \cdot A^{-1.9} \cdot 10^4$	$\frac{\gamma}{G_{(0001)} \cdot c} \cdot 10^4$	$\overline{K_{0001}\omega_1}$
Ti	1.326	6	137.2	0.589	1.80	5.57	236.8
Mg	0.988	7	243.5	1.023	9.06	28.59	
Co	1.063	8	200.6	0.892	3.38	10.09	

Elastic anisotripies data.

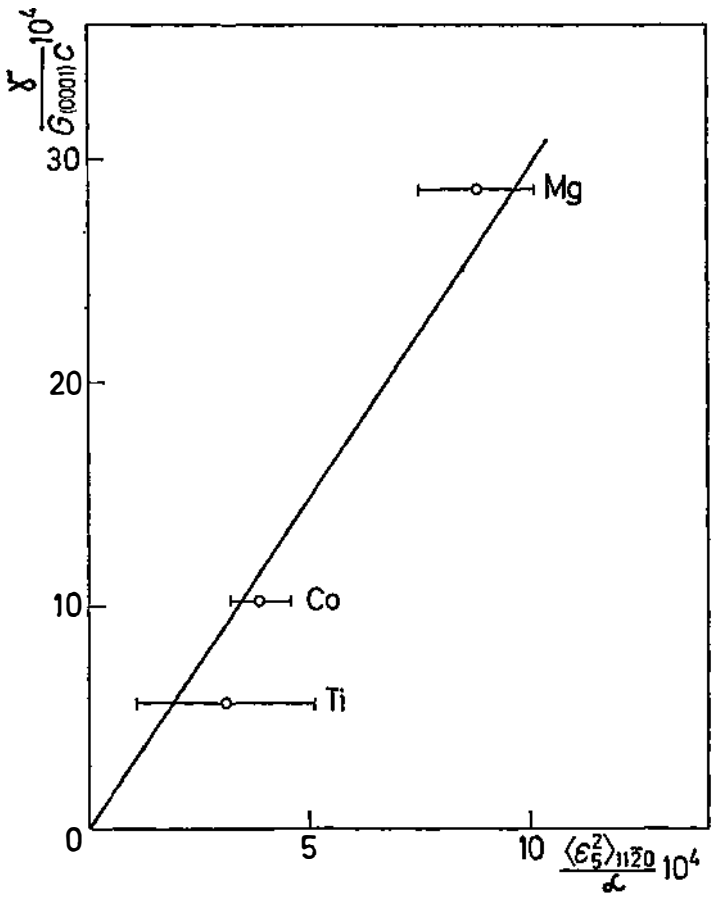

Fig. 1. Stacking fault energies, compiled from literature, for elements Ti, Co and Mg plotted versus the $\frac{\langle\varepsilon_5^2\rangle_{11\bar{2}0}}{a}$ data.

However, $K_{0001}\omega_1$ may depend on elastic anisotropies A of elements, thus Eq. (1) and Eq. (2) should be modified as formulated in (5) and (6)[5]:

$$\gamma = \frac{K_{111}\,\omega_0\,G_{(111)}\,a}{12\,\pi\sqrt{3}}\,A^{-0.45}\,\frac{\langle\varepsilon_5^2\rangle_{111}}{a}, \tag{5}$$

$$\gamma = \frac{K_{0001}\,\omega_1\,G_{(0001)}\,c}{24\,\pi}\,A^{-1.9}\,\frac{\langle\varepsilon_5^2\rangle_{11\bar{2}0}}{a}. \tag{6}$$

$K_{111}\omega_0$ and $K_{0001}\omega_1$ were recalculated by means of the modified Eq. (5) and Eq. (6). The elastic anisotropies of hexagonal elements used in this calculation are given in Table 2. In Fig. 2 the $K_{0001}\omega_1$ values are plotted versus A to obtain

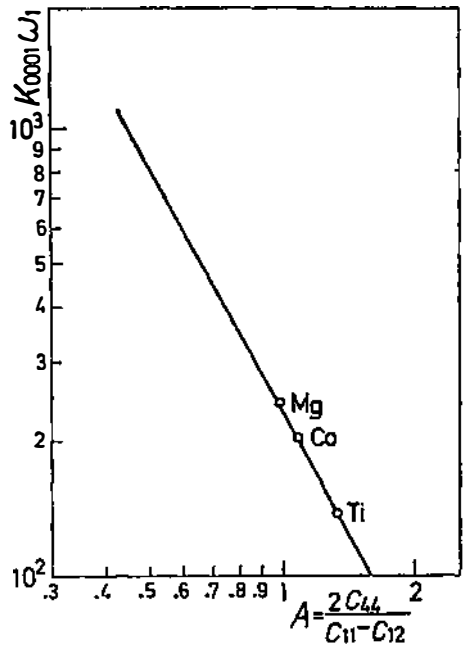

Fig. 2. Variation of $K_{0001}w_1$ with elastic anisotropy.

a variation of $K_{0001}\omega_1$ with elastic anisotropy. The slope of this curve determined the exponent of A in (6). Replotting the data in Fig. 1, Table 1 and Table 2, using Eq. (6), $K_{0001}\omega_1$ computed from the slope of Fig. 3 is 236.8. Comparing Fig. 1 and Fig. 3, it is evident that the data in Fig. 3, obtained using the elastic anisotropy correction factor $A^{-1.9}$, are more linear.

3. *Dependence of SFE upon pressure in FCC and HCP cobalt powder*

Investigating phase transformations in pressed cobalt powder Kirin et al.[4] measured RMSS averaged over the distance of 2 nm, as well as SFP as functions of applied external pressure in the interval from 22.1 to 661.0 MPa. From these experimental data we took the average of RMSS over the distance of 5 nm, in order to make it comparable with the data given in (5). Inserting these data of RMSS and SFP in Eq. (5) and Eq. (6), we calculated the values of SFE for cubic and hexagonal cobalt powder submitted to different pressures. The results are summarized in Tables 3a and 3b, and represented in Figs. 4a and 4b.

4. *Discussion and conclusion*

From Figs. 4a and 4b it is evident that the measurement errors of SFE are great because both RMSS and SFP were measured with considerable errors. Ho-

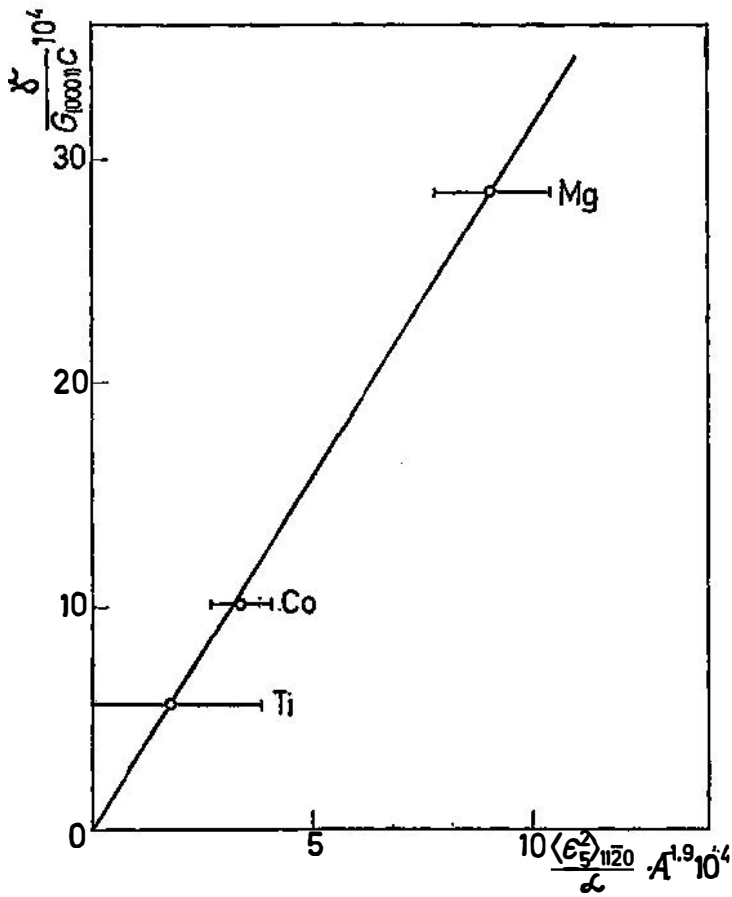

Fig. 3. Stacking fault energies plotted versus $\frac{\langle \varepsilon_5^2 \rangle_{11\bar{2}0}}{\alpha}$ accounting for the effect of elastic anisotropy.

wever, it may be concluded that SFE in HCP cobalt increase with growing pressure, while in FCC cobalt there is a maximum at about 100 MPa, and at higher pressures SFE decrease. This is the consequence of increasing SFP in FCC phase from 0.8×10^{-2} to 5.6×10^{-2} with growing pressure, found in Ref. 4. HCP phase shows relatively high SFP at all pressures, though there is a tendency of SFP decreasing with increasing pressure.

We may regard stacking faults as nuclei for the transition from one close-packed structure (FCC) to the other (HCP) and vice versa. It is obvious that low stacking fault energy means easy transition and that high one characterizes stable structures. Thus, as transformation from the metastable FCC phase to the stable HCP phase takes place with growing pressure, it is to expect that in the HCP phase the stacking fault probability decreases and stacking fault energy increases, while the inverse expectancy appears justified for the FCC phase, this being in agreement with our results.

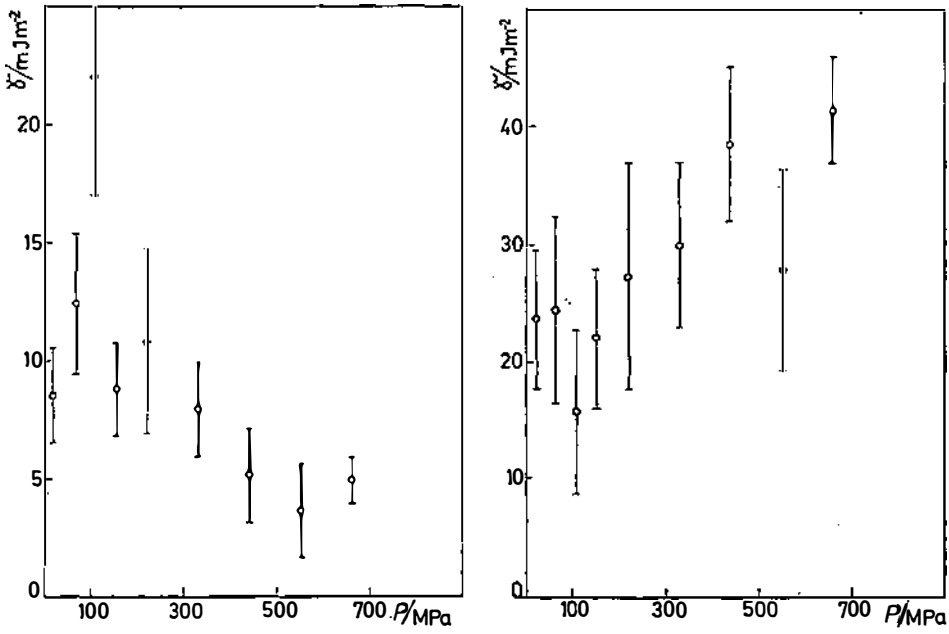

Fig. 4. Stacking fault energies in a) FCC phase of Co, and b) HCP phase of Co, as functions of applied pressure.

TABLE 3.a

P/MPa	$\langle \varepsilon_3^2 \rangle_{111}^{1/2} \cdot 10^3$	$\alpha \cdot 10^2$	γ_{FCC}/mJm^{-2}
22.1	1.9 ± 0.2	1.3 ± 0.1	8.5 ± 2
66.2	2.3 ± 0.2	1.3 ± 0.1	12.4 ± 3
110,0	1.9 ± 0.3	0.50 ± 0.05	22 ± 5
154.5	2.4 ± 0.2	2.0 ± 0.2	8.8 ± 2
221.0	2.6 ± 0.3	1.9 ± 0.2	10.8 ± 4
331.0	3.1 ± 0.2	3.7 ± 0.3	7.9 ± 2
440.0	2.9 ± 0.3	5.0 ± 0.5	5.1 ± 2
552.0	2.4 ± 0.4	4.9 ± 0.5	3.6 ± 2
661.0	3.0 ± 0.3	5.6 ± 0.2	4.9 ± 1

TABLE 3.b

P/MPa	$\langle \varepsilon_3^2 \rangle_{11\bar{2}0}^{1/2} \cdot 10^3$	$\alpha \cdot 10^2$	γ_{HCP} / $\frac{mJ}{m^2}$
22.1	2.1 ± 0.2	1.8 ± 0.1	23.6 ± 6
66.2	2.3 ± 0.2	2.1 ± 0.3	24.3 ± 8
110.0	1.9 ± 0.3	2.2 ± 0.3	15.8 ± 7
154.5	2.4 ± 0.2	2.5 ± 0.2	22.2 ± 6
221.0	2.6 ± 0.3	2.4 ± 0.3	27.2 ± 10
331.0	3.1 ± 0.2	3.1 ± 0.3	29.9 ± 7
440.0	2.9 ± 0.3	2.1 ± 0.3	38.6 ± 14
552.0	2.4 ± 0.4	2.0 ± 0.5	27.8 ± 14
661.0	3.0 ± 0.3	2.1 ± 0.3	41.3 ± 4

Root mean square strains (RMSS), stacking fault probabilities (SFP), and stacking fault energies (SFE) for a) FCC and b) HCP cobalt, as functions of pressure.

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PROCJENA ENERGIJA POGREŠAKA U SLAGANJU U PRAŠKU KOBALTA U OVISNOSTI O TLAKU

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Ranija mjerenja vjerojatnosti pogrešaka u slaganju (SFP) i relativne prosječne deformacije (RMSS) iskorištena su sada za procjenu energija pogrešaka u slaganju (SFE) u metastabilnom prašku kobalta, pri različitim vanjskim tlakovima do 660 MPa. SFE u HCP kobaltu rastu s rastućim tlakom, dok se u FCC kobaltu javlja maksimum na oko 100 MPa, a pri većim tlakovima SFE opadaju.