Elastic Anisotropy and Its Temperature Dependence of the Single Crystals of Fe-19.43%Cr Alloy*

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Rod-form single crystals of Fe-19.43%Cr alloy of the *bcc* type about 3 mm in diameter and 12 cm in length were prepared. The thermal expansion and Young's modulus in the temperature range -150° to 250°C and the rigidity modulus at 20°C of the alloy were measured by means of a dilatometer, a vibrator-controlled oscillator system and the torsion pendulum method, respectively. The results of calculations based on the measured values have shown that the Young's moduli of the single crystals at 20°C in the $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ directions are 14.22×10^5 , 22.23×10^5 and 27.37×10^5 kg/cm², and the rigidity moduli at 20°C are 11.36×10^5 , 7.21×10^5 and 6.43×10^5 kg/cm², respectively; the elastic anisotropy is not very large in all cases. The Young's modulus in the $\langle 111 \rangle$ shows a small minimum at 10°C and a small maximum at about 110°C with increasing temperature, while the Young's moduli in the $\langle 100 \rangle$ and $\langle 110 \rangle$ directions monotonously decrease. The mean temperature coefficients of Young's modulus at $10^{\circ}\sim 110^{\circ}\text{C}$ are -32.77×10^{-5} , -9.85×10^{-5} and $+4.71 \times 10^{-5}$ in the $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ directions, respectively. The calculated value of Young's modulus for the polycrystal agrees fairly well with the measured value for the polycrystal specimen prepared by melting.

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I. Introduction

In a previous paper⁽¹⁾ the present authors and Sawaya carried out measurements of the mean temperature coefficient of Young's modulus at $0^{\circ}\sim 40^{\circ}\text{C}$ for Fe-Cr polycrystal alloys containing 4.7~59.10% Cr. The result that the Fe-19.43%Cr alloy showed the lowest negative value of -6.81×10^{-5} . It was reported from this result that the Elinvar property was revealed in this system⁽²⁾. Therefore, it is a problem of great interest to investigate the variation in the temperature coefficient of elasticity with crystal direction in these Fe-Cr alloys. The present study was carried out so as to examine the temperature dependence of elastic anisotropy in single crystals of the Fe-19.43%Cr alloy with various directions.

II. Experimental Procedure

The alloying materials used were electrolytic iron and electrolytic chromium whose chemical compositions are tabulated in Table 1. For the preparation of specimens,

a wire of 2 mm diameter with a composition of 80.57% Fe and 19.43% Cr was at first prepared, from which single crystal specimens were produced by the Tammann-Bridgman method⁽³⁾. The single crystals with rod axes near to the $\langle 110 \rangle$ direction⁽⁴⁾ were most easily obtainable and the optimum descending rate of the crucible for their growth was 0.07 mm/min. However, since the single crystals of the $\langle 100 \rangle$ and $\langle 111 \rangle$ directions could hardly be obtained by the Tammann-Bridgman method alone, even though the descending rate of the crucible was changed, crystals of a desired directions were produced by adapting Fujiwara's method^{(5)~(8)}. The optimum descending rate of the crucible for development of the two directions was 0.05 mm/min.

The single crystals of about 3 mm diameter thus were cut to the length of 12 cm and used as specimens for Young's modulus measurement. The orientation of the specimen was determined by the light-figure method⁽⁹⁾ after corroding in a 15°C mixture of 99 cc of Fe_3Cl and 1 cc of Br for about 20 min. For measurements of Young's modulus and the rigidity modulus, quasi-isotropic

Table 1 Chemical compositions of iron and chromium used

Metals	Fe (%)	Cu (%)	Al (%)	Si (%)	C (%)	S (%)	P (%)
Electrolytic Fe		0.004	—	—	0.005	0.005	0.004
" Cr	0.11	—	0.06	0.07	0.03	0.02	0.01

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polycrystal specimens about 3 and 0.5 mm in diameter were prepared from the molten alloy which was solidified at such a rate as to permit no crystal growth.

The specimens were all subjected to electropolishing, heating in a vacuum at 1000°C for about 1 hr, and cooling at a rate of 300°C/hr, and then finished off by electropolishing prior to measurement. The orientation distribution of all the single crystal specimens is indicated by the open circles in the stereographic projection⁽¹⁰⁾ diagram of Fig. 1, and the orientations are summarized in Table 2.

Fig. 1 Stereographic projection of the orientations in single crystals of Fe-19.43% Cr alloy.

Table 2 Crystal orientations in single crystals of Fe-19.43% Cr alloy

No.	θ_1 (degr.)	θ_2 (degr.)	θ_3 (degr.)
1	87.24	87.30	3.40
2	80.01	82.45	12.24
3	72.24	85.06	18.17
4	68.39	85.45	21.40
5	69.39	77.36	24.08
6	58.36	82.15	32.34
7	58.15	69.45	39.02
8	46.39	89.09	43.22
9	55.00	61.00	49.15
10	56.00	57.00	51.20

The thermal expansion was measured by the Super-Invar vertical-type dilatometer⁽¹¹⁾ and the horizontal-type dilatometer, and the density was determined by weighing in water. Young's modulus was calculated from the resonance frequency of vibration of a specimen excited by means of a vibrator-controlled oscillator system⁽¹²⁾ and the measured values of the thermal expansion coefficient and the density. The rigidity modulus measurement was carried out at room temperature by the torsional pendulum method⁽¹³⁾.

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III. Results and Discussion

1. Thermal expansion

Three specimens having rod axes nearest to the $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ directions, respectively, were used to measure the thermal expansions in the temperature range of $-150^\circ \sim 250^\circ \text{C}$, the results of which are shown in Fig. 2. As indicated by the figure, the thermal expansions are almost independent of the crystal directions and their expansion curves are nearly straight, with a thermal expansion coefficient of 10.23×10^{-6} .

Fig. 2 Thermal expansion of single crystals in Fe-19.43% Cr alloy.

2. Young's modulus

Young's modulus E was calculated from the resonance frequency of vibration (500~800 Hz) and the measured values of the thermal expansion coefficient and the density (7.72 g/cm³). The temperature dependence of E is illustrated in Fig. 3. As shown in the figure, the value of E is largest in specimen No. 10 near to the $\langle 111 \rangle$ direction and is smallest in specimen No. 1

Fig. 3 Temperature dependence of Young's modulus in single crystals and a polycrystal of Fe-19.43% Cr alloy.

near to the $\langle 100 \rangle$ direction, indicating a comparatively large anisotropy of E . In the specimen with the rod axis near to the $\langle 100 \rangle$ direction, E continuously decreases gradually with rise in temperature, but the rate of decrease in E diminishes with the approach to the $\langle 111 \rangle$ direction and E shows a trend toward a slight increase at temperatures between $-50^\circ \sim 100^\circ \text{C}$ in the specimen near to the $\langle 111 \rangle$ direction.

However, since E in an arbitrary direction cannot be obtained only from these measured values, the following relation⁽¹⁴⁾ for the isometric crystals may be used:

$$\frac{1}{E} = S_{11} - 2(S_{11} - S_{12} - \frac{1}{2}S_{44})(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2) \quad (1)$$

where S_{ij} is the elastic parameter and α_i and α_j are direction cosines of the rod axis with regard to the crystal axis. The orientation function $3\Sigma\alpha_i^2\alpha_j^2$ is 0, 1/4 and 1/3 in the $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ directions, respectively.

Figure 4 shows the relationship between $1/E$ and $3\Sigma\alpha_i^2\alpha_j^2$, in which the measured points lie on a nearly

Fig. 4 Relations between reciprocals of Young's modulus E , rigidity modulus G and orientation function $3(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2)$ in single crystals of Fe-19.43%Cr alloy.

straight line as the evidence of validity of eq. (1). Accordingly, the values of S_{11} and $S_{11} - S_{12} - (1/2)S_{44}$ at various temperatures can be calculated from the measured values of E in eq. (1) using the least square method. The following relation may also be established in the (110) plane containing the three principal axes:

$$\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2 = \frac{1}{4}(1 + 2\cos^2\theta - 3\cos^4\theta) \quad (2)$$

where θ is an angle between the $[001]$ orientation and the rod axis of the specimen. By substituting eq. (2) into eq. (1), the values of E in an arbitrary direction can be calculated. The temperature dependence of the calculated values of S_{11} and $S_{11} - S_{12} - (1/2)S_{44}$, the temperature dependence of E in the three principal directions and the orientation dependence of E in the (110) plane at -150° , 145° and 250°C are shown in Figs. 5, 6 and 7, respectively. As shown in Fig. 5, S_{11}

and $S_{11} - S_{12} - (1/2)S_{44}$ indicate a nearly similar variation with temperature; both of the calculated values increase linearly in the initial stage with increasing temperature and then increase parabolically from the

Fig. 5 Temperature dependence of calculated values of elastic parameters S_{11} and $S_{11} - S_{12} - (1/2)S_{44}$ in single crystals of Fe-19.43%Cr alloy.

Fig. 6 Temperature dependence of calculated values of Young's modulus in three principal directions for single crystals of Fe-19.43%Cr alloy.

Fig. 7 Calculated values of Young's modulus E , rigidity modulus G and temperature coefficient of Young's modulus e in various orientations in the (110) plane of single crystals of Fe-19.43%Cr alloy.

vicinity of 150°C. The value of E at each temperature is highest in the $\langle 111 \rangle$ direction and smallest in the $\langle 100 \rangle$ direction as given in Fig. 6.

The above results agree well with the following general relation for Young's moduli in the three principal directions in the isometric system as in the case of other metals and alloys⁽¹⁵⁾:

$$E_{\langle 111 \rangle} > E_{\langle 110 \rangle} > E_{\langle 100 \rangle} \quad (3)$$

When the temperature is raised, $E_{\langle 100 \rangle}$ initially decreases linearly, but the decrement is accelerated gradually at temperatures above about 145°C. The value of $E_{\langle 110 \rangle}$ decreases rather steeply in the temperature range up to about -100°C, but the decrement becomes appreciably smaller with an increase in temperature and then decreases severely at temperatures higher than about 145°C. $E_{\langle 111 \rangle}$ decreases gradually with a rise in temperature and reaches a minimum value in the vicinity of 10°C, after which the value continuously increases until a maximum value of about 110°C is attained. Thereafter, the value shows a gradual decrease again, augmenting the decrement at temperatures higher than about 145°C. In the range of 10°C ~ 110°C the temperature coefficient of $E_{\langle 111 \rangle}$ turns out positive.

Table 3 Calculated values of Young's modulus E , rigidity modulus G , temperature coefficient of Young's modulus e in the three principal directions of single crystals, and elastic anisotropies $E_{\langle 111 \rangle}/E_{\langle 100 \rangle}$ and $G_{\langle 100 \rangle}/G_{\langle 111 \rangle}$, and volume compressibility κ for Fe-19.43%Cr alloy

	E	G	$E_{\langle 111 \rangle} / E_{\langle 100 \rangle}$	$G_{\langle 100 \rangle} / G_{\langle 111 \rangle}$	$(\times 10^{-5} \text{kg/cm}^2/\text{kg})$	$\begin{matrix} e \\ (\times 10^{-5}) \end{matrix}$		
	$(\times 10^5 \text{kg/cm}^2)$							
	20°C					-150°~10°C	10°~110°C	110°~250°C
$\langle 100 \rangle$	14.22	11.36	—	—	—	-29.20	-32.77	-80.78
$\langle 110 \rangle$	22.23	7.21	—	—	—	-14.26	-9.85	-49.26
$\langle 111 \rangle$	27.37	6.43	—	—	—	-4.74	+4.71	-25.84
Polycrystal	20.20	7.88	—	—	0.0648	-11.72	-9.90	-56.49
—	—	—	1.92	1.77	—	—	—	—

As shown in Fig. 7, the value of E is very low at any given temperature in the $\langle 001 \rangle$ orientation, but with increasing angle from the orientation, it becomes larger gradually and reaches the highest value in the $\langle 111 \rangle$ orientation. Then the value shows a gradual decrease with further increase in angle up to the $\langle 110 \rangle$ orientation. The orientation dependence of the mean temperature coefficient of E at -150°C~10°C, 10°C~110°C and 110°C~250°C is also shown in the figure. It is to be noted that $e_{10^\circ \sim 110^\circ \text{C}}$ is negative from the $\langle 001 \rangle$ orientation to about 44°, beyond which the value turns out positive and the positive value is sustained up to the angle of 64° after reaching the positive maximum value in the $\langle 111 \rangle$ orientation. Thereafter, the value becomes negative again and the negative value is continuously augmented up to the $\langle 110 \rangle$ orientation. Both $e_{-150^\circ \sim 10^\circ \text{C}}$ and $e_{110^\circ \sim 250^\circ \text{C}}$ are negative in the entire range of orientations investigated.

Figure 8 shows the temperature dependence of elastic

anisotropy $E_{\langle 111 \rangle}/E_{\langle 100 \rangle}$, in which the anisotropy increases gradually with a rise in temperature and indicates a slight bend between room temperature and 150°C, followed by a steep increase over 150°C. The values of the elastic anisotropy at -150°, 20°, 110° and 250°C are as small as 1.85, 1.92, 1.98 and 2.17, respectively, which are comparable with those of body-centered cubic metals such as iron⁽¹⁶⁾. Table 3 shows the values of E at room temperature in the three principal directions, the average temperature coefficient of E at -150°C~10°C, 10°C~110°C and 110°C~250°C and the values of elastic anisotropy at room temperature.

Fig. 8 Temperature dependence of calculated values of elastic anisotropy $E_{\langle 111 \rangle}/E_{\langle 100 \rangle}$ in single crystals of Fe-19.43%Cr alloy.

The value of E in the quasi-isotropic polycrystallite has heretofore been calculated by Voigt⁽¹⁴⁾, Reuß⁽¹⁷⁾ and other workers^{(18)~(22)}. Here, the value of E for the polycrystal specimen can be derived from Reuß' equation

$$E_p = \frac{5}{3S_{11} + 2S_{12} + S_{44}} \quad (4)$$

by using the mean value of the strain component S_{ij} on the assumption that the straining condition is equal for all the crystallites. A comparison between the data calculated from the above relation and the measured values of E_p for the quasi-polycrystal specimen slow-cooled after melting is shown in Fig. 6, both being in good agreement. The rigidity modulus of the polycrystal

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specimen measured at room temperature is also listed in Table 3.

3. Volume compressibility

The following relation holds for the volume compressibility κ , E and G :

$$\kappa = \frac{3(3G - E)}{EG} \quad (5)$$

Using the measured values of E and G , κ can be derived from the above relation as given in Table 3.

4. Elastic parameter and elastic constant

Since there is a relation

$$\kappa = 3(S_{11} + 2S_{12}) \quad (6)^{(14)}$$

between κ and S_{ij} , the value of S_{12} can be obtained using the measured values of S_{ij} in Fig. 5 and κ in Table 3. At the same time, the value of S_{44} at 20°C can be calculated from the value of $S_{11} - S_{12} - (1/2)S_{44}$ in Fig. 5 as shown in Table 4. The principal elastic constant C_{ij} can be derived from the following relations :

Table 4 Calculated values of elastic parameter S_{ij} and elastic constant C_{ij} at 20°C of the Fe-19.43% Cr alloy

S_{ij}	($\times 10^{-5}$ cm ² /kg)	C_{ij}	($\times 10^5$ kg/cm ²)
S_{11}	0.0703	C_{11}	22.41
S_{12}	-0.0243	C_{12}	11.84
S_{44}	0.0880	C_{44}	11.36

$$\left. \begin{aligned} C_{11} &= \frac{S_{11} + S_{12}}{(S_{11} - S_{12})(S_{11} + 2S_{12})} , \\ C_{12} &= \frac{-S_{12}}{(S_{11} - S_{12})(S_{11} + 2S_{12})} , \\ C_{44} &= \frac{1}{S_{44}} , \end{aligned} \right\} (7)^{(14)}$$

The values of C_{ij} at 20°C, calculated from the above relations, are tabulated in Table 3, but Cauchy's relation, $C_{12} = C_{44}$ ⁽²³⁾, does not hold for the cubic crystal system⁽²⁴⁾.

5. Rigidity modulus of single crystals

Since the rigidity modulus G and S_{ij} for the principal directions in the isometric system crystal specimen have the following relation :

$$\frac{1}{G} = S_{44} + 4(S_{11} - S_{12} - \frac{1}{2}S_{44})(\alpha_1^2\alpha_2^2 + \alpha_2^2\alpha_3^2 + \alpha_3^2\alpha_1^2) , \quad (8)^{(14)}$$

the values of G for various orientations and temperatures can be calculated by substituting the predetermined values of S_{ij} into the above relation. The results thus obtained are shown in Fig. 7 and Table 3, from which

it is clear that G is largest in the $\langle 100 \rangle$ direction and smallest in the $\langle 111 \rangle$ direction. This tendency is similar to that of pure metals such as iron and nickel in the cubic crystal system⁽²⁵⁾ and Diaflex⁽²⁶⁾. The relationship between $1/G$ and the direction function at 20°C is shown in Fig. 4, and the curves are almost linear. The anisotropy of G , $G_{\langle 100 \rangle}/G_{\langle 111 \rangle}$, is illustrated in Table 3, indicating small values as in the case of E .

As mentioned already, it has been made clear that the temperature coefficient of Young's modulus in single crystals of the Fe-Cr alloy containing 19.43% Cr exhibits the highest positive value of $+4.71 \times 10^{-5}$ in the $\langle 111 \rangle$ direction. It is very interesting to note that the Fe-19.43% Cr alloy exhibits a positive temperature coefficient of Young's modulus at room temperature despite its fairly high magnetic transformation point. The authors will carry out further research to clarify the cause for this phenomenon.

IV. Conclusions

Single crystals of the Fe-19.43% Cr alloy prepared by the Tammann-Bridgman method, and subjected to slow cooling from 1000°C were measured so as to determine the thermal expansion and Young's modulus at $-150^\circ \sim 250^\circ \text{C}$. Their rigidity modulus of the polycrystal specimen was also measured at room temperature. The results obtained are as follows :

(1) The thermal expansion of the single crystals determined at $-150^\circ \sim 250^\circ \text{C}$ is isotropic and the expansion curves are almost linear, the linear coefficient of thermal expansion being 10.23×10^{-6} .

(2) The calculated values of Young's modulus of the single crystals in the three principal directions and of the polycrystal specimen at 20°C are $E_{\langle 100 \rangle} = 14.22 \times 10^5$, $E_{\langle 110 \rangle} = 22.33 \times 10^5$, $E_{\langle 111 \rangle} = 27.37 \times 10^5$ and $E_{\text{poly}} = 20.20 \times 10^5$ kg/cm², among which the value of E_{poly} is almost consistent with the measured one for the quasi-isotropic polycrystal specimen. The value of $E_{\langle 111 \rangle}/E_{\langle 100 \rangle}$ at 20°C is 1.92, approaching the mean value of bcc type materials with rise of temperature.

(3) Young's moduli in the $\langle 100 \rangle$ and $\langle 110 \rangle$ directions decreases linearly with the temperature, but the value in the $\langle 111 \rangle$ direction shows a minimum in the vicinity of 10°C and a maximum at about 110°C. The mean temperature coefficients of Young's modulus in the three principal directions and the polycrystal specimen at $10^\circ \sim 110^\circ \text{C}$ are $e_{\langle 100 \rangle} = -32.77 \times 10^{-5}$, $e_{\langle 110 \rangle} = -9.85 \times 10^{-5}$, $e_{\langle 111 \rangle} = +4.71 \times 10^{-5}$ and $e_{\text{poly}} = -9.90 \times 10^{-5}$, respectively.

(4) The principal elastic parameters at 20°C are $S_{11} = 0.0703 \times 10^{-5}$, $S_{12} = -0.0243 \times 10^{-5}$ and $S_{44} = 0.0880 \times 10^{-5}$ cm²/kg.

(5) The principal elastic constants at 20°C are $C_{11} = 22.41 \times 10^5$, $C_{12} = 11.84 \times 10^5$ and $C_{44} = 11.36 \times 10^5$ kg/cm², where Cauchy's relation $C_{12} = C_{44}$ does not hold.

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(6) The rigidity modulus at 20°C in the three principal directions is calculated to be $G_{\langle 100 \rangle} = 11.36 \times 10^5$, $G_{\langle 110 \rangle} = 7.21 \times 10^5$ and $G_{\langle 111 \rangle} = 6.43 \times 10^5$ kg/cm², the anisotropy $G_{\langle 100 \rangle}/G_{\langle 111 \rangle}$ being 1.77 at 20°C.

(7) The volume compressibility at 20°C is 0.0648×10^{-5} cm²/kg.

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