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SHORT COMMUNICATION

CRYSTALLOGRAPHIC ANGLES AND STANDARD PROJECTIONS OF POLYETHYLENE CRYSTAL

H. C. CHAO and HSUN HU
United States Steel Corporation, Research Laboratory, Monroeville, Pennsylvania 15146

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Owing to its high crystallinity, linear polyethylene has been one of the most widely used materials for the study of orientation phenomena in polymers. The polyethylene crystal is orthorhombic, and has the unit cell dimensions of a = 7.40 Å, b = 4.93 Å, and c = 2.53 Å, the c-axis being the direction of the molecular chains.[1] Based on the crystal structure and the principles of ordinary crystal plasticity, Frank, Keller, and O'Connor[2] were able to predict the deformation behavior of oriented polyethylene as a consequence of specific slip and twinning processes. Numerous studies have since been reported, for example, on the observations of dislocations in polyethylene single crystals of micron dimensions prepared by crystallization from dilute solutions,[3,4] on the crystallographic features of plastic deformation of these single crystals,[5,6] and on the preferred orientations developed in bulk polyethylene specimens by deformation and by subsequent annealing treatments.[7] That polyethylene crystals may undergo polymorphic phase transformations under suitable stress conditions is also known.[2,8]

To facilitate these and similar studies, the interplanar angles of the orthorhombic polyethylene crystal, and the angles between its crystallographic directions, have been calculated by means of a CDC 6500 computer, using the well-known equations.[9]

$$\cos\phi = \frac{\frac{h_1h_2}{a^2} + \frac{k_1k_2}{b^2} + \frac{l_1l_2}{c^2}}{\left[\left(\frac{h_1^2}{a^2} + \frac{k_1^2}{b^2} + \frac{l_1^2}{c^2}\right)\left(\frac{h_2^2}{a^2} + \frac{k_2^2}{b^2} + \frac{l_2^2}{c^2}\right)\right]^{\frac{1}{2}}}$$

and

$$\cos\rho = \frac{a^2u_1u_2 + b^2v_1v_2 + c^2w_1w_2}{\left[\left(a^2u_1^2 + b^2v_1^2 + c^2w_1^2\right)\left(a^2u_2^2 + b^2v_2^2 + c^2w_2^2\right)\right]^{\frac{1}{2}}}$$

where ϕ is the angle between lattice planes $(h_1k_1l_1)$ and $(h_2k_2l_2)$, and ρ is the angle between lattice directions $(u_1v_1w_1)$ and $(u_2v_2w_2)$. The unit cell dimensions a, b, and c were given earlier. These angles, for indices up to 4, are listed in Tables I and II in a brief form.

TABLE I

Angles between planes of polyethylene crystal

Plane Index	(100)	(010)	(001)	(110)	(111)	(112)
(0 0 1)	90.00	90.00	0.00	90.00	31.66	17.14
(0 1 0)	90.00	0.00	90.00	33.67	64.10	75.81
(0 1 1)	90.00	62.83	27.17	67.67	16.92	15.82
(0 1 2)	90.00	75.61	14.39	78.06	21.09	9.40
(0 1 3)	90.00	80.29	9.71	81.93	24.13	10.49
(0 1 4)	90.00	82.69	7.31	83.92	25.86	11.75
(0 2 1)	90.00	44.25	45.75	53.41	24.93	32.60
(0 2 3)	90.00	71.11	18.89	74.37	18.78	10.41
(0 3 1)	90.00	33.01	56.99	45.74	33.90	43.43
(0 3 2)	90.00	52.41	37.59	59.49	19.79	24.93
(0 3 4)	90.00	68.95	21.05	72.61	17.96	11.50
(0 4 1)	90.00	25.97	64.03	41.57	40.05	50.29
(0 4 3)	90.00	55.62	34.38	61.97	18.35	22.01
(1 0 0)	0.00	90.00	90.00	56.33	73.08	80.60
(1 0 1)	71.12	90.00	18.88	79.67	25.90	16.85
(1 0 2)	80.30	90.00	9.70	84.64	27.37	14.19
(1 0 3)	83.50	90.00	6.50	86.40	28.52	14.54
(1 0 4)	85.11	90.00	4.89	87.29	29.21	14.97

TABLE I (continued)

Plane Index	(100)	(010)	(001)	(110)	(111)	(112)
(1 1 0)	56.33	33.67	90.00	0.00	58.34	72.86
(1 1 1)	73.08	64.10	31.66	58.34	0.00	14.52
(1 1 2)	80.60	75.81	17.14	72.86	14.52	0.00
(1 1 3)	83.59	80.35	11.62	78.38	20.04	5.52
(1 1 4)	85.15	82.72	8.76	81.24	22.90	8.37
(1 2 0)	71.58	18.42	90.00	15.25	59.58	73.49
(1 2 1)	76.58	45.84	47.25	44.89	18.26	30.97
(1 2 2)	81.35	63.17	28.41	62.68	8.27	12.64
(1 2 3)	83.85	71.23	19.83	70.90	13.47	5.51
(1 2 4)	85.27	75.66	15.13	75.41	17.47	4.67
(1 3 0)	77.48	12.52	90.00	21.15	60.69	74.05
(1 3 1)	79.45	34.47	57.62	38.04	29.63	41.94
(1 3 2)	82.29	52.81	38.26	54.73	13.72	23.00
(1 3 3)	84.21	62.98	27.73	64.28	11.13	13.17
(1 3 4)	85.44	69.02	21.52	70.00	13.74	8.19
(1 4 0)	80.54	9.46	90.00	24.22	61.40	74.41
(1 4 1)	81.48	27.24	64.33	34.71	36.86	49.00
(1 4 2)	83.20	44.67	46.14	48.89	20.78	31.14
(1 4 3)	84.63	55.79	34.75	58.68	13.54	20.22
(1 4 4)	85.65	62.92	27.49	65.11	12.57	13.65
(2 0 1)	55.64	90.00	34.36	71.76	29.90	28.23
(2 0 3)	77.16	90.00	12.84	82.92	26.55	14.53
(2 1 0)	36.89	53.11	90.00	19.44	60.33	73.87
(2 1 1)	58.69	67.04	40.53	52.21	14.40	24.92
(2 1 2)	71.68	76.35	23.15	68.24	12.25	8.92
(2 1 3)	77.34	80.53	15.91	75.02	17.40	5.64
(2 1 4)	80.38	82.79	12.06	78.63	20.64	6.99
(2 2 1)	64.49	49.73	50.96	39.04	19.30	33.83
(2 2 3)	77.83	71.55	22.35	67.65	9.31	5.21
(2 3 0)	66.05	23.95	90.00	9.72	58.85	73.12
(2 3 1)	69.57	38.20	59.31	32.05	28.44	42.48
(2 3 2)	74.84	53.93	40.11	50.58	10.17	23.37
(2 3 3)	78.54	63.42	29.32	61.15	5.46	12.73
(2 3 4)	80.94	69.22	22.84	67.51	9.86	6.58
(2 4 1)	73.33	30.55	65.19	28.86	35.24	48.78
(2 4 3)	79.35	56.29	35.80	55.64	9.40	19.72
(3 0 1)	44.27	90.00	45.73	66.61	36.62	38.37
(3 0 2)	62.85	90.00	27.15	75.34	27.10	22.35
(3 0 4)	75.62	90.00	14.38	82.08	26.26	14.93

TABLE I (continued)

Plane Index	(100)	(010)	(001)	(110)	(111)	(112)
(3 1 0)	26.58	63.42	90.00	29.75	62.89	75.18
(3 1 1)	47.62	70.29	48.91	49.13	25.46	34.83
(3 1 2)	63.58	77.14	29.83	64.41	15.19	17.01
(3 1 3)	71.38	80.81	20.92	71.94	16.71	10.28
(3 1 4)	75.73	82.92	16.00	76.15	19.30	8.47
(3 2 0)	45.02	44.98	90.00	11.31	59.02	73.21
(3 2 1)	54.41	54.38	55.43	36.16	24.93	38.72
(3 2 2)	65.47	65.46	35.96	54.84	7.61	19.41
(3 2 3)	72.07	72.06	25.81	64.73	7.96	9.58
(3 2 4)	76.05	76.04	19.94	70.46	12.66	4.55
(3 3 1)	60.81	42.94	61.61	28.39	29.95	44.47
(3 3 2)	67.88	55.59	42.77	47.23	11.11	25.63
(3 3 4)	76.54	69.55	24.82	65.18	6.84	7.68
(3 4 0)	63.45	26.55	90.00	7.12	58.61	73.00
(3 4 1)	65.81	34.91	66.45	24.54	35.16	49.47
(3 4 2)	70.31	47.60	48.93	41.58	17.85	31.98
(3 4 3)	74.24	57.08	37.41	52.92	7.02	20.50
(3 4 4)	77.15	63.57	29.84	60.41	4.07	13.00
(4 0 1)	36.18	90.00	53.82	63.41	42.50	45.90
(4 0 3)	65.49	90.00	24.51	76.70	26.46	20.40
(4 1 0)	20.57	69.43	90.00	35.76	64.79	76.17
(4 1 1)	39.42	73.15	55.60	47.96	33.66	42.51
(4 1 2)	56.48	78.04	36.14	61.41	20.19	24.12
(4 1 3)	65.80	81.15	25.96	69.19	17.87	15.45
(4 1 4)	71.27	83.08	20.06	73.84	18.98	11.58
(4 2 1)	46.34	58.79	59.68	35.51	31.02	43.76
(4 2 3)	66.67	72.71	29.68	62.16	10.07	14.58
(4 3 0)	48.39	41.61	90.00	7.94	58.68	73.03
(4 3 1)	53.32	47.74	64.10	27.01	32.92	47.16
(4 3 2)	61.55	57.57	45.84	44.73	15.00	28.94
(4 3 3)	67.92	64.97	34.47	55.91	5.16	17.64
(4 3 4)	72.30	69.99	27.24	63.04	5.89	10.52
(4 4 1)	59.08	39.53	67.93	22.07	36.27	50.80
(4 4 3)	69.38	58.09	39.43	50.57	7.77	22.29

TABLE II

Angles between directions of polyethylene crystal

Dirct. Index	[100]	[010]	[001]	[110]	[111]	[112]
[0 0 1]	90.00	90.00	0.00	90.00	74.12	60.36
[0 1 0]	90.00	0.00	90.00	56.33	57.77	61.19
[0 1 1]	90.00	27.17	62.83	60.44	53.17	49.12
[0 1 2]	90.00	45.75	44.25	67.24	55.38	46.33
[0 1 3]	90.00	56.99	33.01	72.42	58.67	47.37
[0 1 4]	90.00	64.03	25.97	75.95	61.34	49.03
[0 2 1]	90.00	14.39	75.61	57.52	54.23	53.87
[0 2 3]	90.00	37.59	52.41	63.94	53.88	46.88
[0 3 1]	90.00	9.71	80.29	56.87	55.13	56.06
[0 3 2]	90.00	18.89	71.11	58.36	53.62	51.97
[0 3 4]	90.00	34.38	55.62	62.77	53.51	47.39
[0 4 1]	90.00	7.31	82.69	56.64	55.68	57.26
[0 4 3]	90.00	21.05	68.95	58.84	53.42	51.14
[1 0 0]	0.00	90.00	90.00	33.67	36.83	43.67
[1 0 1]	18.88	90.00	71.12	38.05	32.23	32.39
[1 0 2]	34.36	90.00	55.64	46.61	35.39	28.81
[1 0 3]	45.73	90.00	44.27	54.48	41.00	30.79
[1 0 4]	53.82	90.00	36.18	60.58	46.10	34.29
[1 1 0]	33.67	56.33	90.00	0.00	15.88	29.64
[1 1 1]	36.83	57.77	74.12	15.88	0.00	13.76
[1 1 2]	43.67	61.19	60.36	29.64	13.76	0.00
[1 1 3]	50.73	65.06	49.52	40.48	24.60	10.84
[1 1 4]	56.68	68.53	41.30	48.70	32.81	19.05
[1 2 0]	53.11	36.89	90.00	19.44	24.91	34.96
[1 2 1]	53.98	38.42	78.40	22.52	19.35	25.54
[1 2 2]	56.27	42.28	67.68	29.26	19.44	18.92
[1 2 3]	59.26	47.07	58.38	36.58	23.68	16.82
[1 2 4]	62.36	51.82	50.62	43.21	28.99	18.69
[1 3 0]	63.42	26.58	90.00	29.75	33.38	41.01
[1 3 1]	63.75	27.87	81.30	30.88	29.90	34.84
[1 3 2]	64.67	31.22	72.99	33.88	28.53	29.97
[1 3 3]	66.00	35.63	65.35	37.90	29.18	26.86
[1 3 4]	67.56	40.29	58.54	42.22	31.22	25.60
[1 4 0]	69.43	20.57	90.00	35.76	38.69	45.15
[1 4 1]	69.58	21.63	83.15	36.32	36.14	40.60
[1 4 2]	70.02	24.45	76.49	37.90	34.63	36.75
[1 4 3]	70.70	28.26	70.18	40.23	34.20	33.78
[1 4 4]	71.54	32.45	64.34	42.99	34.71	31.80

TABLE II (continued)

Dirct. Index	[100]	[010]	[001]	[110]	[111]	[112]
[2 0 1]	9.70	90.00	80.30	34.88	33.37	37.22
[2 0 3]	27.15	90.00	62.85	42.22	33.16	29.62
[2 1 0]	18.42	71.58	90.00	15.25	21.88	33.01
[2 1 1]	20.53	71.82	80.79	17.76	16.30	24.92
[2 1 2]	25.52	72.51	72.03	23.40	14.73	18.15
[2 1 3]	31.45	73.49	64.05	29.82	17.41	13.97
[2 1 4]	37.26	74.63	57.03	35.96	21.96	13.43
[2 2 1]	34.52	56.71	81.90	8.10	7.79	21.55
[2 2 3]	40.06	59.34	66.89	23.11	7.23	6.53
[2 3 0]	44.98	45.02	90.00	11.31	19.41	31.54
[2 3 1]	45.39	45.43	83.11	13.22	14.26	25.11
[2 3 2]	46.57	46.60	76.40	17.62	11.17	19.16
[2 3 3]	48.32	48.36	70.06	22.81	11.50	14.11
[2 3 4]	50.45	50.48	64.19	28.02	14.49	10.71
[2 4 1]	53.34	37.29	84.14	20.27	21.54	30.03
[2 4 3]	54.99	40.15	72.89	25.68	18.67	21.75
[3 0 1]	6.50	90.00	83.50	34.22	34.28	39.23
[3 0 2]	12.84	90.00	77.16	35.77	32.73	35.40
[3 0 4]	24.51	90.00	65.49	40.78	32.66	30.31
[3 1 0]	12.52	77.48	90.00	21.15	26.23	35.85
[3 1 1]	14.02	77.56	83.65	22.04	22.81	30.65
[3 1 2]	17.65	77.78	77.46	24.44	20.76	26.02
[3 1 3]	22.18	78.13	71.54	27.79	20.36	22.26
[3 1 4]	26.89	78.58	66.01	31.56	21.44	19.67
[3 2 0]	23.95	66.05	90.00	9.72	18.56	31.06
[3 2 1]	24.63	66.19	84.05	11.38	13.77	25.41
[3 2 2]	26.53	66.59	78.23	15.22	10.30	20.03
[3 2 3]	29.27	67.20	72.65	19.82	9.43	15.17
[3 2 4]	32.47	67.99	67.38	24.52	11.38	11.20
[3 3 1]	34.05	56.50	84.58	5.42	10.46	24.22
[3 3 2]	35.15	56.99	79.26	10.74	5.14	18.90
[3 3 4]	38.91	58.78	69.22	20.78	4.89	8.87
[3 4 0]	41.61	48.39	90.00	7.94	17.71	30.59
[3 4 1]	41.85	48.57	85.13	9.31	13.49	25.88
[3 4 2]	42.52	49.10	80.33	12.49	9.93	21.31
[3 4 3]	43.59	49.95	75.66	16.35	7.82	16.97
[3 4 4]	44.95	51.05	71.18	20.37	8.13	13.01
[4 0 1]	4.89	90.00	85.11	33.98	34.83	40.29
[4 0 3]	14.38	90.00	75.62	36.28	32.51	34.56

TABLE II (continued)

Dirct. Index	[100]	[010]	[001]	[110]	[111]	[112]
[4 1 0]	9.46	80.54	90.00	24.22	28.70	37.57
[4 1 1]	10.60	80.58	85.18	24.66	26.22	33.76
[4 1 2]	13.42	80.68	80.43	25.93	24.43	30.25
[4 1 3]	17.00	80.84	75.81	27.85	23.43	27.16
[4 1 4]	20.82	81.04	71.36	30.21	23.27	24.61
[4 2 1]	18.98	71.64	85.36	15.92	18.73	28.86
[4 2 3]	22.80	72.12	76.33	20.37	14.91	21.30
[4 3 0]	26.55	63.45	90.00	7.12	17.37	30.41
[4 3 1]	26.88	63.53	85.63	8.35	13.47	26.15
[4 3 2]	27.84	63.78	81.31	11.22	10.00	21.99
[4 3 3]	29.32	64.17	77.08	14.72	7.51	17.98
[4 3 4]	31.19	64.70	72.99	18.40	6.92	14.22
[4 4 1]	33.89	56.42	85.93	4.07	11.81	25.57
[4 4 3]	35.52	57.16	77.95	12.05	3.84	17.60

For stereographic applications, standard projections of {100} planes and <100> directions have been produced from the computer data by a CALCOMP plotter. The original plots were accurate to 0.5 deg on a 30 cm diameter Wulff net. It was necessary to remove many high-index points selectively to avoid congestion in the projections. Two of these standard projections, namely (100) and [100], are reproduced here in Figures 1 and 2, respectively.

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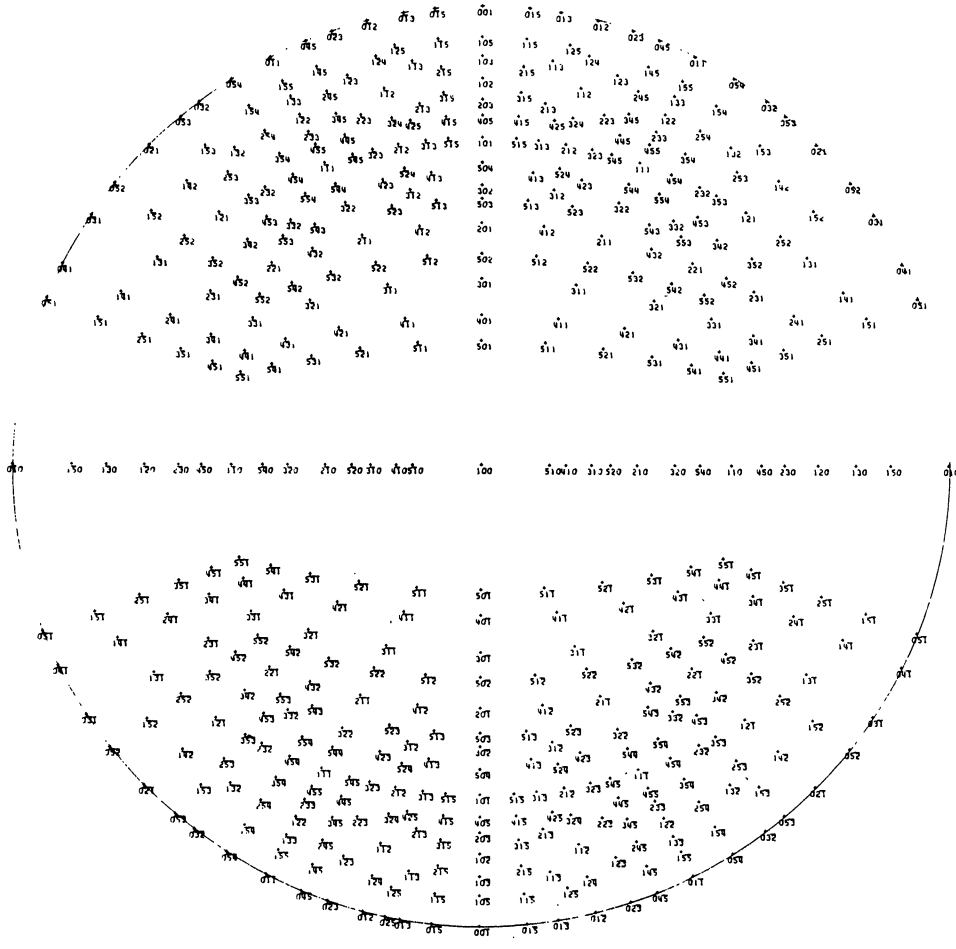

FIGURE 1. Standard projection of (100) plane of polyethylene crystal.

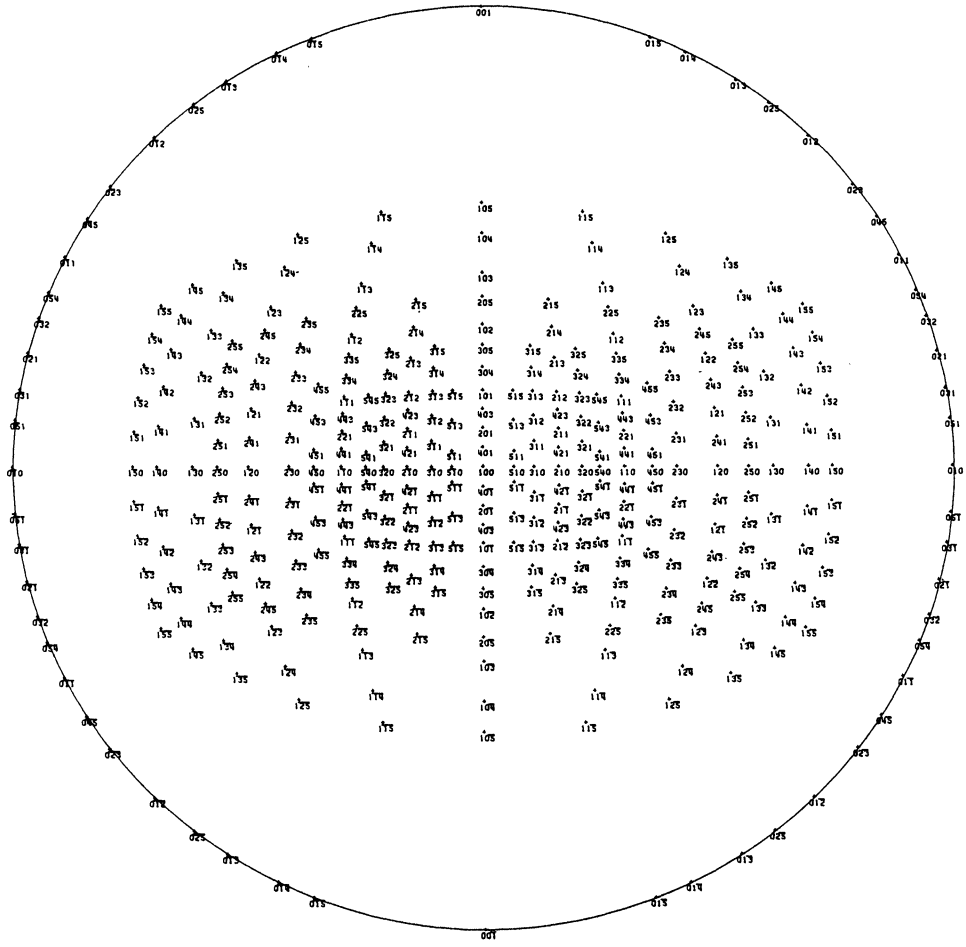

FIGURE 2. Standard projection of [100] direction of polyethylene crystal.