Fig. 6. X-Ray diffraction photograph of PTFE at 12 kbar and 1 bar with sodium chloride used to measure the pressure.
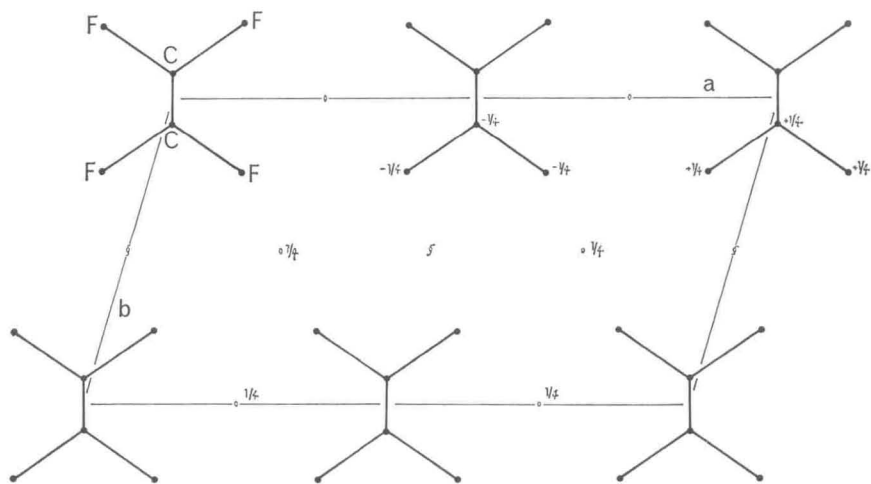

Fig. 7. (001) projection of phase III of PTFE.

between nonbonded atoms is 2.62 Å for two fluorine atoms in the same molecule and 2.70 Å for those in neighboring molecules.

The overwhelming evidence that the molecule has taken on a planar zigzag arrangement is seen in the position of the intense reflections ($\bar{1}11$, 111) on the first layer lines of Figures 3 and 4. These reflections have re-

TABLE II

Atomic Fractional Coordinates for Atoms in the Asymmetric Unit of PTFE Phase III

	x	y	z
Carbon	0.0118	0.0832	0.2500
Fluorine	0.0150	0.2427	0.2500
Fluorine	−0.0810	0.2427	0.2500

TABLE III

Values of hkl, D_{obs}, D_{calc}, F_{calc} I_{obs} for Reflections Appearing on Figure 4

h	k	l	D_{obs}	D_{calc}	F_{calc}	I_{obs}[a]
0	1	0	4.89	4.87	20	VS
2	1	0	2.97	2.96	9	W
0	2	0	2.45	2.43	40	VS
−4	2	0	1.94	1.95	28	M
4	1	0	1.90	1.89	32	M
4	2	0	1.48	1.48	19	S
1	0	1	2.52	2.52	9	W
−1	1	1	2.31	2.31	37	VS
1	1	1	2.17	2.17	37	S
−1	2	1	1.84	1.82	15	M
3	1	1	1.75	1.74	10	M
−5	2	1		1.42	16	
3	2	1	1.42	1.42	13	M
−1	3	1		1.41	11	
0	0	2	1.31	1.31	26	M
0	1	2	1.28	1.27	5	W

[a] VS very strong, S strong, M medium, W weak.

placed the characteristic reflections of the helical structures (106, 107 of phase II and 107, 108 of phase IV; see Figure 2 or Clark and Muus[3]). Application of the theory of Cochran, Crick, and Vand[12] for diffraction from helical structures shows that unwinding the PTFE helix would cause the characteristic helical reflections to approach each other by movement parallel to the meridian and, in the limit of a planar zigzag arrangement, to become coincident.   This has occurred in Figures 3 and 4.

Structure analysis was achieved by a trial-and-error method of solution. As there was only a fiber diagram with few reflections, it was not possible to index reflections from their value of d alone.   It was necessary to postulate trial structures and then to compare both the position and intensity of each reflection on the photograph with that derived from the model structure. It was originally assumed that the specimen in the high pressure cell would have the same degree of preferred orientation as the drawn sample, i.e., with c parallel to the direction of drawing but with random orientation in the plane perpendicular to c.   No model could be made to fit on this assumption. It was found possible, however, to fit a model by allowing preferred orientation in the plane perpendicular to c.