Letters to the Editors

Crystallographic Data for the Hexagonal Crystal System

Investigators in the areas of mechanical metallurgy, crystal growth, and stress analysis have a need for crystallographic data such as the angles between planes. These data are utilized in a standard stereographic projection from which the orientation of a crystal can be determined. Calculations of mechanical properties such as the critical resolved shear stress require values for the angles between planes as well as the angles between directions.

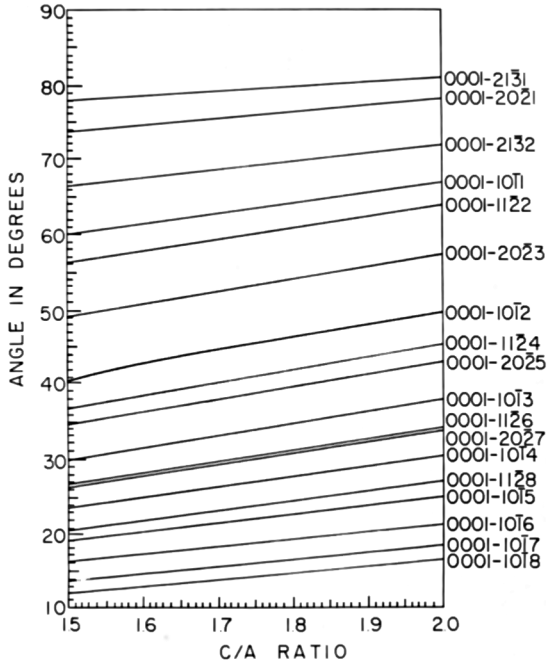

FIG. 1. A nomogram to determine the angles between crystallographic planes for the hexagonal system.

The interplanar angles necessary to construct a (0001) standard projection for magnesium, zinc, and cadmium have been compiled along with a pole figure for zinc (*1*). A similar table for titanium and zirconium together with a projection for titanium have been reported (*2*), and a projection containing only a limited number of poles has been presented for magnesium (*3*). Taylor and Leber (*4*) calculated the angles between planes for the hexagonal system for axial ratios ranging from 1.500 to 2.000 at c/a intervals of 0.050. The angles were computed by means of Peters' tables to 0.001 deg and rounded off to the second decimal place. In addition they presented interplanar angles for beryllium, titanium, zirconium, magnesium, zinc, and cadmium, as well as a new (0001) projection for magnesium.

Since many of the hexagonal elements for which this data is not available are of interest in nuclear engineering applications, it was decided to program these calculations on a high speed digital computer. The angle, θ, between two crystal planes $(HKiL)$ and $(hkil)$ was programmed for the hexagonal system (*5*). The program was designed in a manner similar to that for the tetragonal system which has been previously reported (*6*). The angles were computed for axial ratios from 1.500 to 2.000 at c/a intervals of 0.010 to six decimal places and rounded off to the third decimal place. The computations are presented in Fig. 1 in the form of a nomogram which can be used to determine the angles with an accuracy of the order of one-half of one degree and in Table I for applications where greater accuracy is required. A vertical line is constructed on the nomogram at the specific c/a ratio determined from the lattice parameters of the material. The intersections of this vertical line with each of the curves are projected to the ordinate axis. The readings obtained are the angles between planes identified by the Miller-Bravais indices assigned to each curve.

Table II gives the interplanar angles for hexagonal elements of interest in nuclear engineering using the most recent values of lattice parameters for dysprosium, hafnium, gadolinium, and yttrium (*7–10*). The c/a values used for beryllium and zirconium are the same as those of Taylor and Leber and this allows a direct comparison of the calculated values. Except for the small difference in the second decimal place, the agreement is complete.

The use of a computer can speed the acquisition of crystallographic data necessary to plot pole figures for orientation and plasticity studies. The nomogram is valuable for research involving pure elements as well as alloys for which the variation in c/a ratio can be estimated.

The authors wish to thank the Marquette University Computing Center for the use of their IBM 1620 Computer.

REFERENCES

1. E. I. SALKOVITZ, *Trans. AIME* **191,** 64 (1951); *J. Metals* **3,** 64 (Jan. 1951).

2. C. J. MCHARGUE, *Trans. AIME* **194,** 660 (1952); *J. Metals* **4,** 660 (June 1952).

3. E. SCHMIDT AND W. BOAS, "Plasticity of Crystals" (English translation of "Kristallplastizitat"), Hughes, London, 1950.

4. A. TAYLOR AND S. LEBER, *Trans. AIME* **200,** 190 (1954); *J. Metals.* **6,** 190 (Feb. 1954).

5. C. S. BARRETT, "Structure of Metals." McGraw-Hill, New York, 1952.

6. R. E. FROUNFELKER AND W. M. HIRTHE, *Trans. AIME* **224,** 196 (1962).

TABLE I

ANGLES BETWEEN CRYSTALLOGRAPHIC PLANES FOR THE HEXAGONAL SYSTEM

HKiL	*hkil*	*c/a*									
		1.50	1.51	1.52	1.53	1.54	1.55	1.56	1.57	1.58	1.59
0001	$10\bar{1}8$	12.216	12.295	12.374	12.453	12.532	12.611	12.689	12.768	12.847	12.925
	$10\bar{1}7$	13.898	13.987	14.076	14.165	14.254	14.342	14.431	14.520	14.608	14.697
	$10\bar{1}6$	16.102	16.204	16.305	16.407	16.508	16.610	16.711	16.812	16.913	17.014
	$10\bar{1}5$	19.107	19.225	19.343	19.460	19.578	19.695	19.812	19.929	20.046	20.163
	$10\bar{1}4$	23.413	23.552	23.691	23.830	23.968	24.106	24.244	24.381	24.518	24.655
	$20\bar{2}7$	26.330	26.481	26.632	26.783	26.934	27.084	27.233	27.383	27.531	27.680
	$10\bar{1}3$	30.000	30.165	30.330	30.494	30.657	30.820	30.982	31.144	31.306	31.466
	$20\bar{2}5$	34.715	34.893	35.071	35.248	35.424	35.599	35.774	35.948	36.121	36.293
	$10\bar{1}2$	40.893	41.082	41.269	41.456	41.641	41.825	42.008	42.190	42.372	42.552
	$20\bar{2}3$	49.107	49.295	49.482	49.667	49.851	50.034	50.215	50.395	50.574	50.751
	$10\bar{1}1$	60.000	60.165	60.328	60.489	60.649	60.807	60.963	61.119	61.272	61.424
	$20\bar{2}1$	73.898	73.999	74.099	74.198	74.295	74.392	74.487	74.581	74.674	74.766
	$10\bar{1}0$	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000
	$21\bar{3}2$	66.422	66.561	66.699	66.835	66.970	67.103	67.235	67.365	67.494	67.622
	$21\bar{3}1$	77.690	77.769	77.847	77.924	78.000	78.076	78.150	78.223	78.296	78.367
	$21\bar{3}0$	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000
	$11\bar{2}8$	20.556	20.682	20.807	20.932	21.057	21.181	21.306	21.430	21.554	21.678
	$11\bar{2}6$	26.565	26.718	26.870	27.022	27.173	27.324	27.474	27.625	27.774	27.924
	$11\bar{2}4$	36.870	37.053	37.235	37.416	37.596	37.776	37.954	38.132	38.309	38.485
	$11\bar{2}2$	56.310	56.485	56.659	56.832	57.002	57.172	57.339	57.505	57.670	57.833
	$11\bar{2}0$	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000
$10\bar{1}0$	$21\bar{3}0$	19.107	19.107	19.107	19.107	19.107	19.107	19.107	19.107	19.107	19.107
	$11\bar{2}0$	30.000	30.000	30.000	30.000	30.000	30.000	30.000	30.000	30.000	30.000
	$01\bar{1}0$	60.000	60.000	60.000	60.000	60.000	60.000	60.000	60.000	60.000	60.000

HKiL	*hkil*	*c/a*									
		1.60	1.61	1.62	1.63	1.64	1.65	1.66	1.67	1.68	1.69
0001	$10\bar{1}8$	13.004	13.082	13.161	13.239	13.318	13.396	13.474	13.552	13.630	13.709
	$10\bar{1}7$	14.785	14.873	14.962	15.050	15.138	15.226	15.314	15.402	15.490	15.577
	$10\bar{1}6$	17.115	17.215	17.316	17.416	17.517	17.617	17.717	17.817	17.917	18.017
	$10\bar{1}5$	20.279	20.396	20.512	20.628	20.744	20.859	20.975	21.090	21.205	21.320
	$10\bar{1}4$	24.791	24.927	25.063	25.199	25.334	25.469	25.604	25.738	25.872	26.006
	$20\bar{2}7$	27.829	27.976	28.123	28.270	28.416	28.562	28.708	28.853	28.998	29.142
	$10\bar{1}3$	31.626	31.786	31.945	32.104	32.262	32.419	32.576	32.732	32.888	33.043
	$20\bar{2}5$	36.465	36.635	36.806	36.975	37.143	37.311	37.478	37.644	37.810	37.975
	$10\bar{1}2$	42.731	42.909	43.085	43.261	43.436	43.610	43.783	43.955	44.126	44.296
	$20\bar{2}3$	50.927	51.101	51.275	51.447	51.617	51.787	51.955	52.122	52.287	52.452
	$10\bar{1}1$	61.575	61.724	61.872	62.018	62.163	62.307	62.449	62.590	62.729	62.868
	$20\bar{2}1$	74.857	74.946	75.035	75.123	75.210	75.295	75.380	75.464	75.546	75.629
	$10\bar{1}0$	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000
	$21\bar{3}2$	67.748	67.872	67.996	68.118	68.239	68.359	68.477	68.594	68.710	68.825
	$21\bar{3}1$	78.438	78.508	78.577	78.645	78.713	78.779	78.845	78.910	78.975	79.038
	$21\bar{3}0$	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000
	$11\bar{2}8$	21.801	21.925	22.048	22.171	22.294	22.416	22.538	22.661	22.782	22.904
	$11\bar{2}6$	28.072	28.221	28.369	28.517	28.664	28.811	28.957	29.103	29.249	29.394
	$11\bar{2}4$	38.660	38.834	39.007	39.180	39.352	39.523	39.693	39.862	40.030	40.198
	$11\bar{2}2$	57.995	58.155	58.314	58.471	58.627	58.782	58.935	59.087	59.237	59.387
	$11\bar{2}0$	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000

TABLE I—*Continued*

HKiL	*hkil*	*c/a*									
		1.60	1.61	1.62	1.63	1.64	1.65	1.66	1.67	1.68	1.69
$10\bar{1}0$	$21\bar{3}0$	19.107	19.107	19.107	19.107	19.107	19.107	19.107	19.107	19.107	19.107
	$11\bar{2}0$	30.000	30.000	30.000	30.000	30.000	30.000	30.000	30.000	30.000	30.000
	$01\bar{1}0$	60.000	60.000	60.000	60.000	60.000	60.000	60.000	60.000	60.000	60.000

HKiL	*hkil*	*c/a*									
		1.70	1.71	1.72	1.73	1.74	1.75	1.76	1.77	1.78	1.79
0001	$10\bar{1}8$	13.787	13.865	13.942	14.020	14.098	14.176	14.254	14.331	14.409	14.486
	$10\bar{1}7$	15.665	15.753	15.840	15.927	16.015	16.102	16.189	16.276	16.364	16.450
	$10\bar{1}6$	18.116	18.216	18.315	18.415	18.514	18.613	18.712	18.811	18.909	19.008
	$10\bar{1}5$	21.435	21.549	21.664	21.778	21.892	22.006	22.120	22.233	22.346	22.459
	$10\bar{1}4$	26.139	26.273	26.405	26.538	26.670	26.802	26.934	27.065	27.196	27.327
	$20\bar{2}7$	29.286	29.430	29.573	29.716	29.858	30.000	30.142	30.283	30.423	30.564
	$10\bar{1}3$	33.198	33.352	33.506	33.659	33.811	33.963	34.115	34.266	34.416	34.566
	$20\bar{2}5$	38.139	38.302	38.465	38.627	38.788	38.948	39.108	39.267	39.425	39.583
	$10\bar{1}2$	44.465	44.633	44.800	44.966	45.131	45.295	45.459	45.621	45.782	45.943
	$20\bar{2}3$	52.615	52.777	52.938	53.098	53.256	53.413	53.569	53.724	53.878	54.031
	$10\bar{1}1$	63.004	63.140	63.275	63.408	63.540	63.670	63.800	63.928	64.056	64.182
	$20\bar{2}1$	75.710	75.790	75.869	75.948	76.025	76.102	76.178	76.253	76.327	76.401
	$10\bar{1}0$	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000
	$21\bar{3}2$	68.939	69.051	69.163	69.273	69.382	69.490	69.597	69.703	69.807	69.911
	$21\bar{3}1$	79.101	79.164	79.225	79.286	79.346	79.406	79.464	79.523	79.580	79.637
	$21\bar{3}0$	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000
	$11\bar{2}8$	23.026	23.147	23.268	23.388	23.509	23.629	23.750	23.869	23.989	24.109
	$11\bar{2}6$	29.539	29.683	29.827	29.971	30.114	30.256	30.399	30.541	30.682	30.823
	$11\bar{2}4$	40.365	40.530	40.696	40.859	41.023	41.186	41.348	41.509	41.669	41.829
	$11\bar{2}2$	59.534	59.681	59.826	59.971	60.113	60.255	60.396	60.535	60.673	60.810
	$11\bar{2}0$	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000
$10\bar{1}0$	$21\bar{3}0$	19.107	19.107	19.107	19.107	19.107	19.107	19.107	19.107	19.107	19.107
	$11\bar{2}0$	30.000	30.000	30.000	30.000	30.000	30.000	30.000	30.000	30.000	30.000
	$01\bar{1}0$	60.000	60.000	60.000	60.000	60.000	60.000	60.000	60.000	60.000	60.000

HKiL	*hkil*	*c/a*									
		1.80	1.81	1.82	1.83	1.84	1.85	1.86	1.87	1.88	1.89
0001	$10\bar{1}8$	14.564	14.641	14.719	14.796	14.873	14.951	15.028	15.105	15.182	15.259
	$10\bar{1}7$	16.537	16.624	16.711	16.798	16.884	16.971	17.057	17.143	17.230	17.316
	$10\bar{1}6$	19.107	19.205	19.303	19.401	19.499	19.597	19.695	19.793	19.890	19.988
	$10\bar{1}5$	22.572	22.685	22.798	22.910	23.022	23.134	23.246	23.358	23.469	23.580
	$10\bar{1}4$	27.457	27.587	27.717	27.846	27.976	28.104	28.233	28.361	28.489	28.617
	$20\bar{2}7$	30.704	30.843	30.982	31.121	31.259	31.397	31.535	31.672	31.809	31.945
	$10\bar{1}3$	34.715	34.864	35.012	35.160	35.307	35.453	35.599	35.745	35.890	36.034
	$20\bar{2}5$	39.740	39.896	40.051	40.206	40.360	40.513	40.666	40.818	40.969	41.119
	$10\bar{1}2$	46.102	46.261	46.418	46.575	46.731	46.886	47.040	47.193	47.345	47.497
	$20\bar{2}3$	54.182	54.333	54.482	54.631	54.778	54.924	55.069	55.213	55.356	55.498
	$10\bar{1}1$	64.307	64.430	64.553	64.675	64.795	64.915	65.033	65.150	65.267	65.382
	$20\bar{2}1$	76.474	76.546	76.617	76.688	76.757	76.826	76.895	76.963	77.030	77.096
	$10\bar{1}0$	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000

TABLE I—*Continued*

HKiL	*hkil*	*c/a*									
		1.80	1.81	1.82	1.83	1.84	1.85	1.86	1.87	1.88	1.89
0001	$21\bar{3}2$	70.014	70.116	70.216	70.316	70.415	70.513	70.610	70.706	70.801	70.895
	$21\bar{3}1$	79.693	79.749	79.804	79.859	79.913	79.966	80.019	80.071	80.123	80.174
	$21\bar{3}0$	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000
	$11\bar{2}8$	24.228	24.347	24.466	24.584	24.702	24.821	24.938	25.056	25.174	25.291
	$11\bar{2}6$	30.964	31.104	31.244	31.383	31.522	31.661	31.799	31.937	32.074	32.211
	$11\bar{2}4$	41.987	42.145	42.302	42.459	42.614	42.769	42.923	43.076	43.229	43.380
	$11\bar{2}2$	60.945	61.080	61.213	61.346	61.477	61.607	61.736	61.864	61.991	62.117
	$11\bar{2}0$	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000
$10\bar{1}0$	$21\bar{3}0$	19.107	19.107	19.107	19.107	19.107	19.107	19.107	19.107	19.107	19.107
	$11\bar{2}0$	30.000	30.000	30.000	30.000	30.000	30.000	30.000	30.000	30.000	30.000
	$01\bar{1}0$	60.000	60.000	60.000	60.000	60.000	60.000	60.000	60.000	60.000	60.000

HKiL	*hkil*	*c/a*										
		1.90	1.91	1.92	1.93	1.94	1.95	1.96	1.97	1.98	1.99	2.00
0001	$10\bar{1}8$	15.336	15.413	15.490	15.566	15.643	15.720	15.796	15.873	15.949	16.026	16.102
	$10\bar{1}7$	17.402	17.488	17.574	17.660	17.746	17.831	17.917	18.002	18.088	18.173	18.258
	$10\bar{1}6$	20.085	20.182	20.279	20.376	20.473	20.570	20.667	20.763	20.859	20.956	21.052
	$10\bar{1}5$	23.691	23.802	23.913	24.023	24.134	24.244	24.354	24.463	24.573	24.682	24.791
	$10\bar{1}4$	28.744	28.871	28.998	29.124	29.250	29.376	29.501	29.626	29.751	29.876	30.000
	$20\bar{2}7$	32.081	32.217	32.352	32.486	32.621	32.755	32.888	33.021	33.154	33.286	33.418
	$10\bar{1}3$	36.178	36.322	36.465	36.607	36.749	36.890	37.031	37.171	37.311	37.450	37.589
	$20\bar{2}5$	41.269	41.418	41.567	41.715	41.862	42.008	42.154	42.299	42.444	42.587	42.731
	$10\bar{1}2$	47.648	47.797	47.946	48.094	48.241	48.388	48.533	48.678	48.821	48.964	49.107
	$20\bar{2}3$	55.639	55.779	55.918	56.056	56.193	56.330	56.465	56.599	56.732	56.864	56.996
	$10\bar{1}1$	65.496	65.610	65.722	65.833	65.944	66.053	66.162	66.269	66.376	66.482	66.587
	$20\bar{2}1$	77.161	77.226	77.291	77.355	77.418	77.480	77.542	77.603	77.664	77.724	77.784
	$10\bar{1}0$	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000
	$21\bar{3}2$	70.988	71.081	71.172	71.263	71.353	71.442	71.530	71.618	71.704	71.790	71.875
	$21\bar{2}1$	80.225	80.275	80.325	80.374	80.423	80.471	80.519	80.566	80.613	80.659	80.705
	$21\bar{3}0$	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000
	$11\bar{2}8$	25.408	25.524	25.641	25.757	25.873	25.989	26.105	26.220	26.335	26.450	26.565
	$11\bar{2}6$	32.347	32.484	32.619	32.755	32.889	33.024	33.158	33.292	33.425	33.558	33.690
	$11\bar{2}4$	43.531	43.681	43.831	43.980	44.128	44.275	44.421	44.567	44.712	44.856	45.000
	$11\bar{2}2$	62.241	62.365	62.488	62.610	62.731	62.850	62.969	63.087	63.204	63.320	63.435
	$11\bar{2}0$	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000	90.000
$10\bar{1}0$	$21\bar{3}0$	19.107	19.107	19.107	19.107	19.107	19.107	19.107	19.107	19.107	19.107	19.107
	$11\bar{2}0$	30.000	30.000	30.000	30.000	30.000	30.000	30.000	30.000	30.000	30.000	30.000
	$01\bar{1}0$	60.000	60.000	60.000	60.000	60.000	60.000	60.000	60.000	60.000	60.000	60.000

TABLE II

ANGLES BETWEEN CRYSTALLOGRAPHIC PLANES FOR HEXAGONAL ELEMENTS

HKiL	*hkil*	Dy	Hf	Be	Gd	Y	Zr
		c/a					
		1.5790	1.5822	1.5847	1.5870	1.5880	1.5893
0001	$10\bar{1}8$	12.839	12.864	12.884	12.902	12.910	12.920
	$10\bar{1}7$	14.599	14.628	14.650	14.670	14.679	14.690
	$10\bar{1}6$	16.903	16.935	16.960	16.984	16.994	17.007
	$10\bar{1}5$	20.035	20.072	20.101	20.128	20.140	20.155
	$10\bar{1}4$	24.504	24.548	24.582	24.614	24.627	24.645
	$20\bar{2}7$	27.517	27.564	27.601	27.635	27.650	27.670
	$10\bar{1}3$	31.289	31.341	31.381	31.418	31.434	31.455
	$20\bar{2}5$	36.104	36.159	36.202	36.242	36.259	36.281
	$10\bar{1}2$	42.353	42.411	42.456	42.498	42.516	42.539
	$20\bar{2}3$	50.556	50.613	50.657	50.698	50.716	50.739
	$10\bar{1}1$	61.257	61.306	61.344	61.379	61.394	61.414
	$20\bar{2}1$	74.665	74.694	74.717	74.738	74.748	74.759
	$10\bar{1}0$	90.000	90.000	90.000	90.000	90.000	90.000
	$21\bar{3}2$	67.481	67.522	67.554	67.583	67.596	67.613
	$21\bar{3}1$	78.288	78.311	78.329	78.346	78.353	78.362
	$21\bar{3}0$	90.000	90.000	90.000	90.000	90.000	90.000
	$11\bar{2}8$	21.542	21.581	21.612	21.641	21.653	21.669
	$11\bar{2}6$	27.759	27.807	27.845	27.879	27.894	27.913
	$11\bar{2}4$	38.291	38.348	38.392	38.432	38.450	38.472
	$11\bar{2}2$	57.653	57.706	57.747	57.784	57.800	57.822
	$11\bar{2}0$	90.000	90.000	90.000	90.000	90.000	90.000
$10\bar{1}0$	$21\bar{3}0$	19.107	19.107	19.107	19.107	19.107	19.107
	$11\bar{2}0$	30.000	30.000	30.000	30.000	30.000	30.000
	$01\bar{1}0$	60.000	60.000	60.000	60.000	60.000	60.000

7. KLEMM AND BOMMER, *Z. anorg. Chem.* **231,** 150 (1937).
8. SWANSON AND FUYAT, NBS Circular 539, Vol. III (1953).
9. KLEMM AND BOMMER, *Z. anorg. Chem.* **231,** 150 (1937).
10. QUILL, *Z. anorg. u. allgem. Chem.* **208,** 59 (1932).

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Received November 30, 1961
Revised July 18, 1962

On the Possibility of Using Model Experiments to Study Shielding Problems

The Method

It is a well-known fact that it is possible to study the penetration of gamma radiation theoretically only in the simplest cases. For more complicated configurations it is necessary to make full scale experiments which are both expensive and time consuming. One hitherto untried possibility for simplifying the problem is to perform some kind of model experiment. The purpose of this paper is to discuss this method.

In the following we will deal with concrete shields. This is the case which has the greatest practical importance. In concrete the gamma radiation is attenuated almost entirely by Compton absorption, at least for those energies which are of interest in connection with shielding problems. An obvious way to decrease the dimensions of a shield is to increase the cross section of the Compton absorption by making the shield of some heavier element, for example, iron. Such as iron shield will constitute a good model of the concrete shield. It is evident, however, that a model experiment of this type gives no real gain. An iron shield having the same attenuation as a concrete shield is thinner but has the same weight and is more expensive.

The only possibility to decrease the size of the model further is to decrease the energy of the radiation source. In many practical shielding problems the gamma radiation of 6–8 Mev energy has maximum penetrability and hence it determines the dimensions of the shield. If it is possible to make a model experiment using a radiation source emitting 2–3 Mev gamma radiation, it would be of great importance. An iron model of a thick concrete shield would then be of a reasonable size. Furthermore, there is the great advantage that one is not limited to work with a reactor or an accel-