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Supplementary material to the article

Mössbauer Synchrotron and X-ray Studies of Ultrathin $YFeO_3$ Films

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1. XRD powder diffraction

XRD powder diffraction patterns were calculated by VESTA software (Visualization for Electronic Structural Analysis) [1,2] using *CIF (*Crystallographic Interchange *File)* files for orthorhombic $YFeO_3$ from the paper:[3], for hexagonal $YFeO_3$ from [4] and for Al_2O_3 from [5].

Notice that in this paper, the identification of reflections (h k l) is adopted for the case a<b<c, where a,b,c are the parameters of the crystal lattice.

XRD pattern for the orthorhombic $YFeO_3$

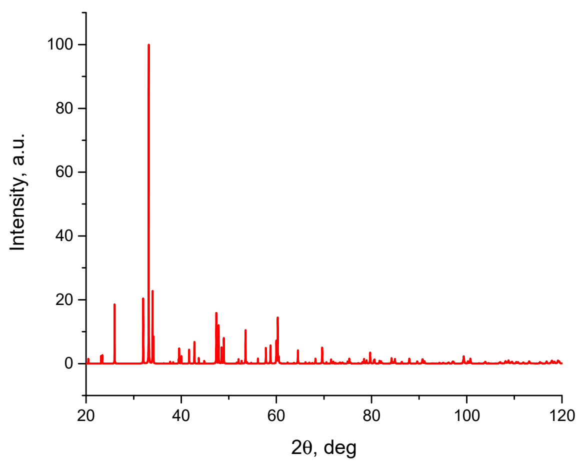

Table S1. Numerical data for reflections from orthorhombic $YFeO_3$. The highlighted lines mark the reflections observable for our epitaxial films in the used geometries.

h	k	l	d. Å	F_{real}	F_{imag}	|F|	2θ. deg
0	1	0	5.58770	-	-	-	14.984
1	0	1	4.33217	15.7468	0.90312	15.7727	20.48426
1	1	0	3.8355	21.94806	-5.53789	22.6359	23.17137
0	0	2	3.79755	-34.73988	4.7597	35.0644	23.40621
1	1	1	3.42371	-53.21165	-3.32456	53.3154	26.00446
0	2	0	2.79385	143.5066	17.86577	144.614	32.00883
1	1	2	2.69859	-167.265	-19.85184	168.439	33.17076
2	0	0	2.63715	166.04965	20.37891	167.296	33.96676

0	2	1	2.62208	-71.8385	-5.97269	72.0864	34.16801
1	2	0	2.46887	-9.47027	0.57132	9.48749	36.3601
2	1	0	2.38488	-21.74638	0.55643	21.7535	37.68783
1	2	1	2.34793	-14.52858	0.45063	14.5356	38.30385
1	0	3	2.28238	35.49293	-0.60942	35.4982	39.44891
2	1	1	2.27535	47.5836	1.77012	47.6165	39.57589
0	2	2	2.25043	-47.74689	7.22929	48.2911	40.03266
2	0	2	2.16609	-69.14248	4.7279	69.3039	41.6625
1	1	3	2.11291	63.44149	3.42967	63.5341	42.76177
1	2	2	2.06989	-33.704	-0.83807	33.7144	43.69575
2	1	2	2.01964	-24.31607	-0.83815	24.3305	44.84111
2	2	0	1.91775	162.27302	17.98853	163.267	47.36479
0	0	4	1.89878	201.31333	20.91512	202.397	47.86759
0	2	3	1.87603	95.13238	6.17174	95.3324	48.4849
2	2	1	1.85939	-85.53697	-5.96824	85.7449	48.94706
1	2	3	1.76755	-20.20219	-0.67786	20.2136	51.67234
1	3	0	1.75627	-55.03638	-10.67637	56.0624	52.02883
2	1	3	1.73595	-31.25658	-1.69993	31.3028	52.68443
3	0	1	1.71281	14.80521	2.50573	15.0158	53.45228
2	2	2	1.71185	7.88459	7.71557	11.0316	53.48453
1	3	1	1.71112	-112.22096	-7.75244	112.488	53.50927
1	1	4	1.70167	20.62239	-5.56408	21.3598	53.83034
3	1	0	1.67705	25.71475	-5.85441	26.3728	54.68609
3	1	1	1.6376	-48.42781	-3.22136	48.5348	56.11804
1	3	2	1.59406	-86.76128	-14.90429	88.0321	57.79322
0	2	4	1.57042	136.32656	18.03533	137.514	58.74736
2	0	4	1.54091	156.93517	20.54276	158.274	59.98623
3	1	2	1.53411	-159.33826	-19.72344	160.554	60.27964
2	2	3	1.52868	60.49871	5.81943	60.778	60.51608
2	3	0	1.52137	21.78075	1.72439	21.8489	60.83763
1	2	4	1.50512	10.51037	0.70111	10.5337	61.56554
2	3	1	1.49174	10.89876	0.53461	10.9119	62.17879
3	2	0	1.488	39.78686	2.14608	39.8447	62.3525
2	1	4	1.48547	2.99505	0.6935	3.0743	62.47086
3	2	1	1.46024	13.7692	1.666	13.8696	63.67525
1	0	5	1.45969	28.25161	1.05391	28.2713	63.70214
3	0	3	1.44406	-31.55837	-2.65117	31.6695	64.47434
1	3	3	1.44304	96.39345	7.69491	96.7001	64.52509
1	1	5	1.41229	-33.68721	-3.27059	33.8456	66.10703
2	3	2	1.41226	-4.19987	-1.57018	4.48379	66.10901
3	1	3	1.39812	16.07461	2.95909	16.3447	66.86451
0	4	0	1.39693	53.41014	11.62788	54.6612	66.92937
3	2	2	1.38544	-23.74422	-2.01397	23.8295	67.55836
0	4	1	1.37388	-92.30054	-7.91553	92.6393	68.20459
1	4	0	1.35037	42.03329	1.19496	42.0503	69.56124
2	2	4	1.3493	118.08534	17.86176	119.429	69.6243
0	2	5	1.33452	-48.85827	-5.87049	49.2097	70.5087
1	4	1	1.32952	-4.44587	-0.16428	4.4489	70.81412
4	0	0	1.31858	127.84605	19.86058	129.38	71.49137
0	4	2	1.31104	63.38937	13.90452	64.8964	71.96625
2	3	3	1.30403	-27.70231	-0.71341	27.7115	72.41398

1	2	5	1.29375	-18.28985	0.33395	18.2929	73.08192
1	3	4	1.28931	-34.67303	-10.60966	36.2599	73.37472
4	1	0	1.28333	39.1528	1.68652	39.1891	73.77327
3	2	3	1.28283	-2.37875	-1.55347	2.84108	73.80653
2	1	5	1.28121	36.12789	1.80616	36.173	73.91574
3	3	0	1.2785	-3.96596	-10.39621	11.127	74.09825
1	4	2	1.27232	0.38693	-0.78219	0.87266	74.51907
0	0	6	1.26585	-66.30089	4.42802	66.4486	74.96529
4	1	1	1.26539	37.61912	3.18857	37.754	74.99716
3	3	1	1.26076	-74.87497	-7.19871	75.2202	75.32023
3	1	4	1.25697	32.32245	-5.78907	32.8368	75.58745
4	0	2	1.24563	-17.96749	5.63605	18.8307	76.399
2	4	0	1.23443	34.21645	11.51329	36.1015	77.21887
0	4	3	1.22309	58.4162	7.60751	58.9095	78.07
2	4	1	1.21845	-78.60102	-7.65025	78.9724	78.42472
4	1	2	1.21578	1.51215	-1.2653	1.9717	78.62962
3	3	2	1.21168	-63.0231	-14.70523	64.716	78.94798
1	1	6	1.20208	-122.03176	-19.89148	123.642	79.70385
4	2	0	1.19244	88.88002	17.30218	90.5485	80.47872
1	4	3	1.19147	9.25481	0.22221	9.25748	80.55754
2	2	5	1.19074	-75.26483	-6.04465	75.5072	80.61745
2	3	4	1.18727	12.4294	1.64936	12.5384	80.90148
4	2	1	1.17801	-64.71802	-5.53458	64.9542	81.67189
2	4	2	1.17397	57.08486	13.86384	58.7443	82.01355
3	2	4	1.17121	27.7845	2.0818	27.8624	82.2485
0	2	6	1.15302	-10.26404	7.48591	12.7039	83.83624
3	0	5	1.14942	9.05474	2.43105	9.37541	84.15939
1	3	5	1.1489	-92.85344	-7.78198	93.179	84.20542
4	1	3	1.14467	-44.62872	-3.29352	44.7501	84.58954
3	3	3	1.14124	83.75606	7.34228	84.0773	84.90315
2	0	6	1.14119	-31.02746	4.97587	31.4239	84.90738
4	2	2	1.13767	3.21157	8.1003	8.71373	85.23176
1	2	6	1.12642	-3.74417	-0.64164	3.79875	86.28974
3	1	5	1.12584	-50.28565	-3.35602	50.3975	86.34474
0	4	4	1.12522	39.49589	11.58466	41.1598	86.40452
2	1	6	1.11811	1.86721	-0.6307	1.97085	87.09056
2	4	3	1.10956	94.28223	7.88053	94.611	87.93241
1	4	4	1.10045	17.92805	0.99413	17.9556	88.85101
3	4	0	1.09371	25.87366	2.60606	26.0046	89.54566
1	5	0	1.09327	-86.20961	-17.05099	87.8797	89.59146
4	0	4	1.08304	110.81863	19.83476	112.58	90.67074
3	4	1	1.08254	-9.79265	-0.47091	9.80396	90.72438
1	5	1	1.08211	-77.74898	-6.75986	78.0423	90.77018
4	2	3	1.07877	63.34246	5.55804	63.5858	91.13081
4	3	0	1.07619	21.98663	3.19531	22.2176	91.41123
2	3	5	1.07494	1.10073	0.44281	1.18646	91.54812
4	3	1	1.06555	18.73262	1.07118	18.7632	92.59067
4	1	4	1.06326	16.99359	1.48158	17.0581	92.84962
3	2	5	1.06297	17.29963	1.72378	17.3853	92.8816
1	0	7	1.06276	8.64686	-0.67489	8.67316	92.90573
3	3	4	1.06051	-16.03467	-10.56267	19.2011	93.16234

2	2	6	1.05646	-17.25126	7.52371	18.8205	93.62739
3	4	2	1.05099	-41.37631	-2.81048	41.4717	94.26438
1	5	2	1.0506	9.90429	-8.23423	12.8801	94.31031
5	0	1	1.04483	45.50776	4.30183	45.7106	94.99452
1	1	7	1.04404	40.12214	3.40623	40.2665	95.0889
5	1	0	1.03655	36.09459	-6.35012	36.6489	95.99817
4	3	2	1.03542	-39.56776	-3.4259	39.7158	96.1376
2	4	4	1.03495	30.9642	11.54561	33.0467	96.19579
2	5	0	1.02896	7.95206	1.40119	8.07457	96.94106
0	4	5	1.02823	-91.3544	-8.07368	91.7105	97.03278
5	1	1	1.02703	-20.28853	-2.72302	20.4705	97.18473
1	3	6	1.02691	-55.77732	-14.80332	57.7083	97.19988
2	5	1	1.01965	-2.47685	-0.88665	2.63077	98.13005
0	2	7	1.01142	64.16724	6.12737	64.4591	99.21078
3	1	6	1.01034	-112.33736	-19.62454	114.039	99.35436
4	2	4	1.00982	80.76755	17.32216	82.6042	99.42404
1	4	5	1.00923	-1.23809	-0.13453	1.24537	99.50285
3	4	3	1.00402	7.03384	0.44222	7.04773	100.20783
1	5	3	1.00368	72.98294	6.74379	73.2939	100.25437
5	1	2	0.99997	-106.92534	-18.94645	108.591	100.76523
1	2	7	0.99332	-8.80668	-0.6272	8.82899	101.69644
2	5	2	0.99315	-4.73139	-1.35811	4.92245	101.72044
4	3	3	0.99042	2.02332	-0.80383	2.17715	102.10929
2	1	7	0.98761	-22.61353	-1.71558	22.6785	102.5141
5	2	0	0.98686	33.73357	3.26872	33.8916	102.62224
4	1	5	0.98031	28.56289	3.13469	28.7344	103.58359
5	2	1	0.97864	31.43283	2.84268	31.5611	103.83308
3	3	5	0.97815	-60.56848	-7.12499	60.9861	103.90508
5	0	3	0.97372	-49.13712	-4.37806	49.3318	104.57442
2	3	6	0.97307	-14.18198	-1.68374	14.2816	104.67345
3	2	6	0.96417	-26.49207	-2.11125	26.5761	106.05532
5	1	3	0.95926	40.18256	3.01006	40.2951	106.83675
4	4	0	0.95888	24.52162	11.56981	27.114	106.89909
2	4	5	0.95799	-61.05666	-7.53202	61.5195	107.04216
5	2	2	0.95514	-28.15335	-3.19949	28.3346	107.50629
2	5	3	0.95324	17.20628	1.09313	17.241	107.81817
4	4	1	0.95132	-77.29003	-7.25601	77.6299	108.13513
0	0	8	0.94939	108.67518	20.6323	110.616	108.45833
3	4	4	0.94773	30.91555	2.70552	31.0337	108.73696
1	5	4	0.94744	-82.75015	-17.12803	84.5042	108.78534
2	2	7	0.94435	51.54204	5.8526	51.8733	109.31158
3	5	0	0.94313	-93.37118	-17.09344	94.9229	109.52061
0	4	6	0.93802	43.49338	13.83909	45.642	110.40968
4	2	5	0.93796	-55.53652	-5.52253	55.8104	110.41937
4	3	4	0.93626	28.82984	3.30751	29.0189	110.71881
3	5	1	0.93594	-55.97446	-6.25503	56.3229	110.77616
0	6	0	0.93128	-18.1727	6.0399	19.1501	111.61097
4	4	2	0.9297	53.43123	13.88422	55.2057	111.89924
0	6	1	0.92436	-26.39808	-4.04177	26.7057	112.8845
1	4	6	0.92353	-21.86681	-1.08615	21.8938	113.04101
3	0	7	0.92333	-22.62333	-2.61875	22.7744	113.07708

XRD pattern for the hexagonal $YFeO_3$

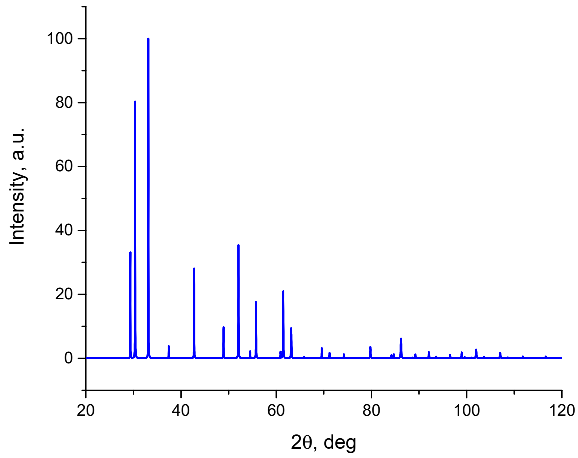

Table S2. Numerical data for reflections from hexagonal $YFeO_3$. The highlighted lines mark the reflections observable for our epitaxial films in the used geometries.

h	k	l	D	F(real)	F(imag)	∣F∣	2θ
0	0	-1	11.759	0	0	0	7.51192
0	0	1	11.759	0	0	0	7.51192
0	0	2	5.8795	24.48098	-2.41352	24.5997	15.05638
1	1	0	3.03966	42.46843	0.82088	42.4764	29.35939
1	0	1	2.94293	-43.77209	-5.40336	44.1043	30.34724
0	0	4	2.93975	97.26827	9.99803	97.7808	30.38085
1	0	2	2.70016	61.32862	6.82651	61.7074	33.151
1	0	3	2.40203	13.27334	5.2224	14.2638	37.40887
1	0	4	2.11316	47.79589	0.62412	47.8	42.7566
0	0	6	1.95983	-9.77284	-3.0503	10.2378	46.28781
1	0	5	1.86006	-34.12666	-5.32415	34.5395	48.92827
1	1	0	1.75495	102.39196	9.7291	102.853	52.07099
1	1	2	1.68164	19.63952	-2.17799	19.7599	54.52446
1	0	6	1.64715	57.48018	6.2842	57.8227	55.76435
2	2	0	1.51983	31.77729	0.78375	31.787	60.90584
2	0	1	1.50729	28.19212	4.9604	28.6252	61.46706
1	1	4	1.50687	68.48864	9.20432	69.1044	61.48639
2	0	2	1.47146	47.39916	6.30252	47.8163	63.13326
1	0	7	1.47027	28.10942	5.2467	28.5949	63.19037
0	0	8	1.46988	62.36821	9.01529	63.0164	63.2094
2	0	3	1.41704	-11.04268	-4.79416	12.0385	65.85763
2	0	4	1.35008	35.11703	0.60091	35.1222	69.57818
1	0	8	1.32328	26.57498	-0.10377	26.5752	71.19837
1	1	6	1.30739	-1.64286	-2.76832	3.2191	72.19846
2	0	5	1.27648	23.77082	4.88769	24.2681	74.23526
2	0	6	1.20101	44.71277	5.79914	45.0873	79.78849
1	0	9	1.20036	-13.17124	-5.04045	14.1028	79.84026
0	0	10	1.1759	4.42521	-3.59919	5.70409	81.84987
2	1	0	1.14888	26.22867	0.74776	26.2393	84.20722
2	1	1	1.14344	-20.46204	-4.55815	20.9636	84.70126

2	1	2	1.12756	38.75309	5.82356	39.1882	86.18118
2	0	7	1.12702	-20.54429	-4.81658	21.1014	86.23225
1	1	8	1.12684	48.39326	8.2964	49.0993	86.24927
2	1	3	1.1025	8.74599	4.40528	9.7928	88.64254
1	0	10	1.0967	31.14445	5.21212	31.5776	89.23629
2	1	4	1.07007	28.52433	0.57773	28.5302	92.08524
2	0	8	1.05658	21.83575	-0.07318	21.8359	93.61333
2	1	5	1.03229	22.17621	2.84745	22.3583	96.52445
3	0	0	1.01322	59.07386	8.26882	59.6498	98.97166
3	0	1	1.00948	-1E-6	0	9.4362E-7	99.46983
1	0	11	1.00845	18.40595	5.02387	19.0793	99.60762
3	0	2	0.9985	16.07999	-1.7784	16.178	100.96885
2	1	6	0.99114	36.63421	5.35601	37.0237	102.00709
3	0	3	0.98098	0	0	9.0604E-15	103.48477
0	0	12	0.97992	43.42571	7.8553	44.1305	103.64203
1	1	10	0.97688	5.20134	-3.28094	6.14967	104.09604

XRD pattern for the Al_2O_3 (Sapphire).

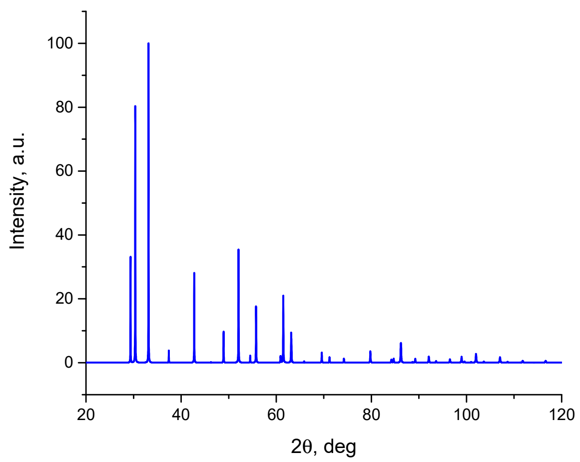

Table S3. Numerical data for reflections from Al_2O_3 (Sapphire). The highlighted lines mark the reflections observable for our *r*-Al_2O_3 substrate in the used geometries.

h	k	l	d. Å	F_{real}	F_{imag}	|F|	2θ. deg
-1	0	2	3,47813	-47,76522	-0,89898	47,7737	25,5906
1	0	4	2,55017	-84,18907	-2,40899	84,2235	35,1624
1	1	0	2,3777	62,62173	2,66746	62,6785	37,80601
0	0	6	2,16517	-11,19556	1,66989	11,3194	41,68101
1	1	3	2,08419	75,96208	0,48577	75,9636	43,38076
2	0	2	1,96288	-14,53728	-0,73991	14,5561	46,21183
-2	0	4	1,73907	-96,05282	-2,56806	96,0871	52,58284
1	1	6	1,60088	107,29859	2,52617	107,328	57,52379
2	1	1	1,54552	-17,86554	-0,14922	17,8662	59,78939
1	2	2	1,51371	-21,21051	-0,79501	21,2254	61,17834
0	1	8	1,51068	44,29455	1,24637	44,3121	61,31452
2	1	4	1,40368	-79,7776	-2,51295	79,8172	66,56525
3	0	0	1,37277	144,17299	3,47488	144,215	68,2676

1	2	5	1,33528	-15,29066	-0,14922	15,2914	70,46278
2	0	8	1,27508	24,39986	1,08731	24,4241	74,33027
1	0	10	1,23892	-88,13153	-2,98267	88,182	76,88774
1	1	9	1,23388	-45,58566	-0,48577	45,5882	77,26027
2	1	7	1,19262	13,47779	0,14922	13,4786	80,46453
2	2	0	1,18885	57,37006	2,68439	57,4328	80,77204
-3	0	6	1,15938	14,48348	1,71876	14,5851	83,27346
3	0	6	1,15938	14,48348	1,71876	14,5851	83,27346
2	2	3	1,14643	-38,01213	-0,43993	38,0147	84,42909
1	3	1	1,13782	8,85743	0,10338	8,85804	85,21819
3	1	2	1,12495	-33,28723	-0,97101	33,3014	86,43009
1	2	8	1,1237	27,55919	1,14241	27,5829	86,54971
0	2	10	1,09872	-67,66345	-2,82361	67,7223	89,02876
0	0	12	1,08258	59,0643	1,05617	59,0737	90,71997
1	3	4	1,07752	-52,53927	-2,33696	52,5912	91,26715
3	1	5	1,04563	8,06652	0,10338	8,06718	94,899
2	2	6	1,04209	76,32079	2,50925	76,362	95,32347
0	4	2	1,01688	-39,55255	-1,0919	39,5676	98,49036
2	1	10	0,99738	-66,74666	-2,87871	66,8087	101,12551
1	1	12	0,98526	-9,08994	0,19989	9,09213	102,85443
4	0	4	0,98144	-39,93773	-2,21607	39,9992	103,41623
1	3	7	0,97274	-7,4676	-0,10338	7,46832	104,72384
3	2	1	0,94231	12,6515	0,18097	12,6528	109,66117
1	2	11	0,94085	10,415	0,14922	10,4161	109,91493
2	3	2	0,93496	-7,39243	-0,67308	7,42301	110,94995
3	1	8	0,93425	35,87141	1,3184	35,8956	111,07784
2	2	9	0,91767	29,94693	0,43993	29,9502	114,15492
3	2	4	0,90719	-65,31769	-2,63489	65,3708	116,22726
0	1	14	0,90523	53,9922	2,59133	54,0543	116,62722
4	1	0	0,89869	50,54978	2,9053	50,6332	117,99308
2	3	5	0,88792	11,92896	0,18097	11,9303	120,34583
4	1	3	0,87994	30,77571	-4,99309	31,1781	122,1847
1	4	3	0,87994	26,67412	0,40818	26,6772	122,1847
-4	0	8	0,86953	41,18973	1,43929	41,2149	124,71852
1	3	10	0,8578	-68,81153	-3,0547	68,8793	127,79059

2. Diffraction curves for epitaxial film/substrate case

It is incorrect to use powder diffraction patterns for epitaxial films. Therefore, the diffraction curves for the film/substrate case were calculated based on the dynamic theory of X-ray diffraction. The calculation algorithm is based on the paper [6].

The calculations of the XRD patterns for epitaxial $YFeO_3$/*r*-Al_2O_3 films have been performed for the three models. The crystal lattice parameters are taken from the corresponding CIF files. The results are shown below.

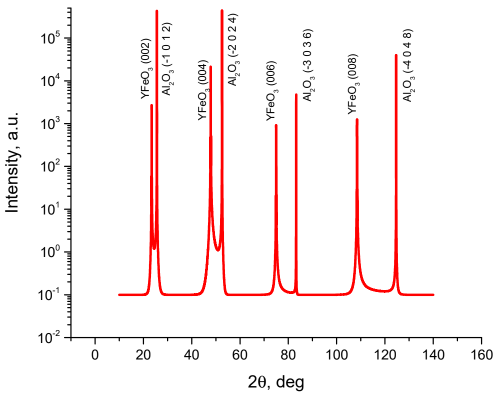

Figure S1. 100 nm layer of (001) orthorhombic $YFeO_3$ on *r*-Al_2O_3.

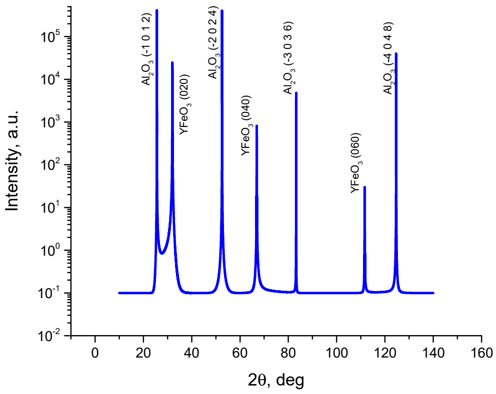

Figure S2. 100 nm layer of (010) orthorhombic $YFeO_3$ on *r*-Al_2O_3.

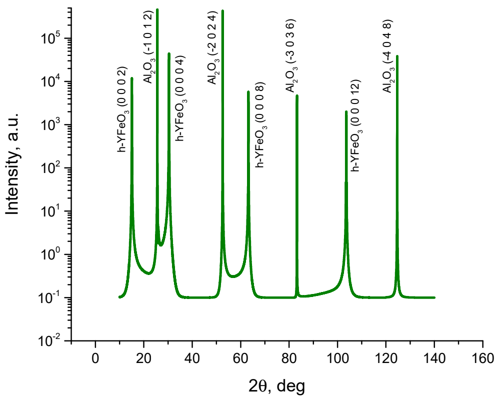

Figure S3. 100 nm layer of hexagonal (0 0 0 1) $YFeO_3$ on *r*-Al_2O_3.

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