Transverse CPGE

Low-Frequency Peak

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Original POSCAR

```
Primitive Cell
 1.000000
   7.4800       0       0
        0  8.6160  -2.8040
        0  8.6160   2.8040
 S  Ta
 8  12
 direct
  0.8270000000  0.8476000000  0.0728000000
  0.1730000000  0.9272000000  0.1524000000
  0.8270000000  0.4272000000  0.6524000000
  0.1730000000  0.3476000000  0.5728000000
  0.5843000000  0.2692000000  0.5000000000
  0.4157000000  0.5000000000  0.7308000000
  0.5843000000  0.0000000000  0.2308000000
  0.4157000000  0.7692000000  0.0000000000
  0.7189600000  0.5895100000  0.0781100000
  0.2810400000  0.9218900000  0.4104900000
  0.7189600000  0.4218900000  0.9104900000
  0.2810400000  0.0895100000  0.5781100000
  0.1045500000  0.6546000000  0.1308000000
  0.8954500000  0.8692000000  0.3454000000
  0.1045500000  0.3692000000  0.8454000000
  0.8954500000  0.1546000000  0.6308000000
  0.6551000000  0.0263000000  0.4737000000
  0.3449000000  0.5263000000  0.9737000000
  0.9942000000  0.7609000000  0.7391000000
  0.0058000000  0.2609000000  0.2391000000
```

From the provided POSCAR data, the lattice vectors are given by:

$$\boldsymbol{a} = \begin{bmatrix} 7.4800 \\ 0 \\ 0 \end{bmatrix}, \quad \boldsymbol{b} = \begin{bmatrix} 0 \\ 8.6160 \\ -2.8040 \end{bmatrix}, \quad \boldsymbol{c} = \begin{bmatrix} 0 \\ 8.6160 \\ 2.8040 \end{bmatrix}$$

Where $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$ are the lattice vectors of the unit cell.

The lengths of the lattice vectors are:

$$| \boldsymbol{a} | = 7.4800 \, A^{\circ}$$
$$| \boldsymbol{b} | = 9.0608 \, A^{\circ}$$
$$| \boldsymbol{c} | = 9.0608 \, A^{\circ}$$

So, the values for $\boldsymbol{a}$, $\boldsymbol{b}$, and $\boldsymbol{c}$ in the unit cell are 7.4800 Å, 9.0608 Å, and 9.0608 Å respectively.

Effects of tilted velocity

$$\mathcal{H}(\mathbf{k}) = \sum_{i=x,y,z} \left(\nu_i^t \hbar k_i + \nu_i \hbar k_i \sigma_i\right) - \mu$$

The CPGE tensor for the tilted term in the Weyl Hamiltonian as follows

$$\beta_{ij} = \frac{3e^3\,\mathrm{sgn}(\mathcal{C})}{\pi h^2}\left[\frac{\nu_i^t \nu_j^t}{\nu_j^2}\frac{1}{{\mathcal{W}_\mathcal{T}}^2}\sum_{n=1}^{2}(-1)^n \sin(\gamma_n)\cos(\gamma_n)^3\right]$$

with

$$\gamma_n = \arcsin\{\frac{1}{\mathcal{W}_\mathcal{T}}[\frac{2|\mu|}{\hbar\omega} + (-1)^{n+1}]\}$$

The maximum value of β_{ij} is profoundly affected by

$$\begin{cases} \dfrac{\nu_i^t}{\nu_i} = \dfrac{\nu_j^t}{\nu_j} \\ \dfrac{\nu_k^t}{\nu_k} = 0 \end{cases}$$

Thus, we notice that under these conditions, the maximum value of β_{ij} is given by:

$$\beta_{ij} = \frac{9\sqrt{3}e^3\,\mathrm{sgn}(C)}{32\pi^2h^2}\frac{\nu_i^t}{\nu_j^t}$$

The maximum value of β_{xz} is profoundly affected by

$$\begin{cases} \dfrac{\nu_x^t}{\nu_x} = \dfrac{\nu_y^t}{\nu_y} \\ \dfrac{\nu_z^t}{\nu_z} = 0 \end{cases}$$

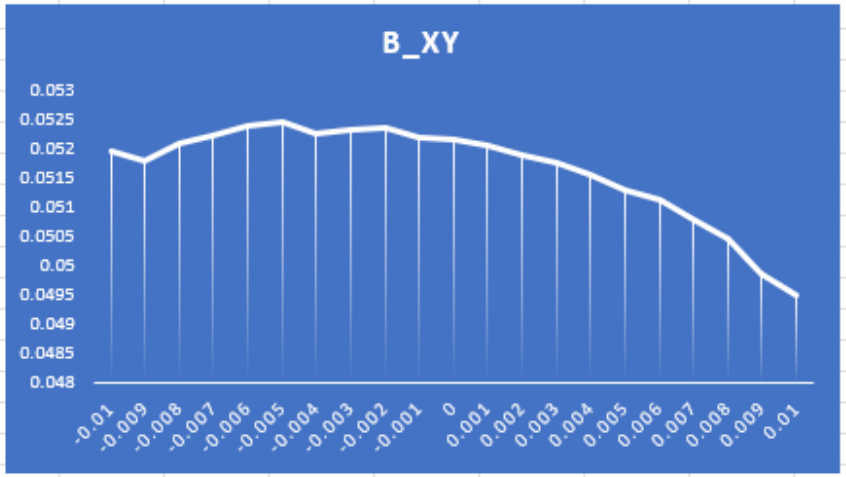
Thus, we notice that under these conditions, the maximum value of β_{xy} is given by:

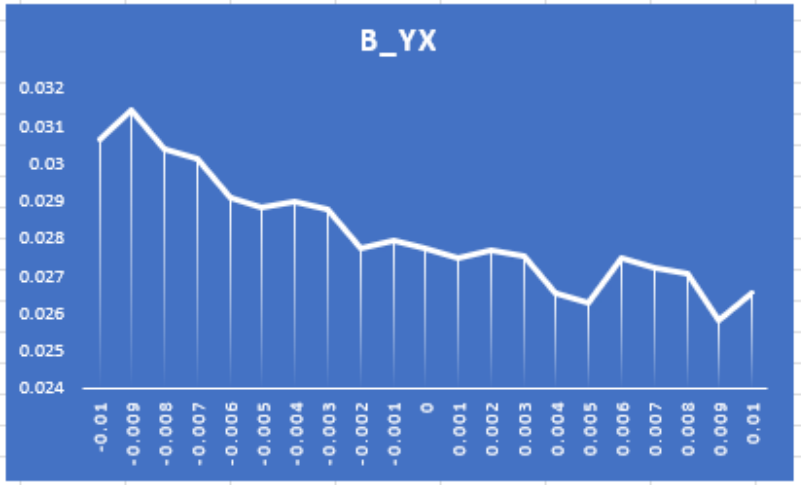
$$\beta_{xy} = \frac{9\sqrt{3}e^3\,\mathrm{sgn}(C)}{32\pi^2h^2}\frac{\nu_x^t}{\nu_y^t}$$

X

D=(b'-b)/b	-0.01	-0.009	-0.008	-0.007	-0.006	-0.005	-0.004	-0.003	-0.002	-0.001	0	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.01
v^t_x	0.60504	0.60153	0.59197	0.58275	0.57283	0.56312	0.5577	0.54742	0.53626	0.52996	0.51809	0.50593	0.49832	0.48487	0.47038	0.45576	0.44657	0.43101	0.41494	0.39791	0.38175
v^t_y	0.51214	0.50457	0.50624	0.50343	0.50503	0.50215	0.49421	0.49125	0.49284	0.48484	0.47947	0.47646	0.46844	0.46302	0.46225	0.4568	0.44173	0.43626	0.42833	0.42744	0.4148
v^t_z	-0.3414	-0.3328	-0.3407	-0.3402	-0.3483	-0.3482	-0.3446	-0.3447	-0.3528	-0.3493	-0.3473	-0.3476	-0.3441	-0.3424	-0.348	-0.3464	-0.334	-0.333	-0.33	-0.3363	-0.3272
v_x	0.68705	0.67787	0.6896	0.69017	0.70178	0.70211	0.69755	0.69739	0.70867	0.70394	0.70073	0.70017	0.69534	0.69192	0.70034	0.69693	0.67759	0.674	0.66771	0.67632	0.65772
v_y	0.5276	0.5278	0.52675	0.52423	0.52308	0.52053	0.51959	0.51697	0.51569	0.51486	0.51108	0.50865	0.50793	0.50446	0.50229	0.49894	0.49648	0.49321	0.48908	0.48669	0.48159
v_z	0.54098	0.54286	0.54735	0.5492	0.55445	0.55688	0.55555	-0.559	-0.5659	-0.5662	-0.5678	0.57331	0.5755	0.57919	0.58578	0.59072	0.5907	0.59693	0.60172	0.60946	0.61469
d_x	0.03446	0.9082	1.16111	0.8493	1.14771	0.93359	0.47635	0.45382	1.03191	0.91348	0.16523	0.67513	1.02623	0.7871	1.01093	1.08178	0.80824	1.26653	0.81945	1.5979	1.40638
d_y	0.07527	-0.8905	-1.105	-1.0377	-1.3427	-1.4115	-0.2513	-0.5702	-1.2772	-0.5758	0.07706	-0.8505	-0.6955	-0.5904	-0.7715	-0.9713	-0.0886	-0.6453	0.02216	-0.6772	-0.3031
d_z	-0.433	-1.4369	-1.0913	-1.3169	-1.0301	-1.3708	-0.2394	0.77135	0.8066	0.06508	-0.0741	-0.8998	-0.5893	-0.8042	-0.5208	-0.9332	-0.737	-1.3518	-0.9788	-1.1198	-1.4271

D=b'-b	-0.01	-0.009	-0.008	-0.007	-0.006	-0.005	-0.004	-0.003	-0.002	-0.001	0	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.01
B^t_xy	0.05193	0.05178	0.052059	0.052196	0.052365	0.052433	0.05225	0.052295	0.052327	0.052164	0.052125	0.052046	0.051877	0.051748	0.051528	0.051284	0.051108	0.050787	0.050448	0.04985	0.049482
B^t_yx	0.030623	0.031392	0.030375	0.030115	0.029092	0.02882	0.028991	0.028737	0.027709	0.027905	0.027728	0.027467	0.027681	0.027506	0.026505	0.026285	0.027439	0.027195	0.027067	0.025815	0.026528





$$\mathcal{H}(\mathbf{k}) = \sum_{i=x,y,z} \left[\nu_i^t \hbar k_i + \left(\nu_i \hbar k_i + \delta_i \hbar^2 k_i^2\right) \sigma_i\right] - \mu$$

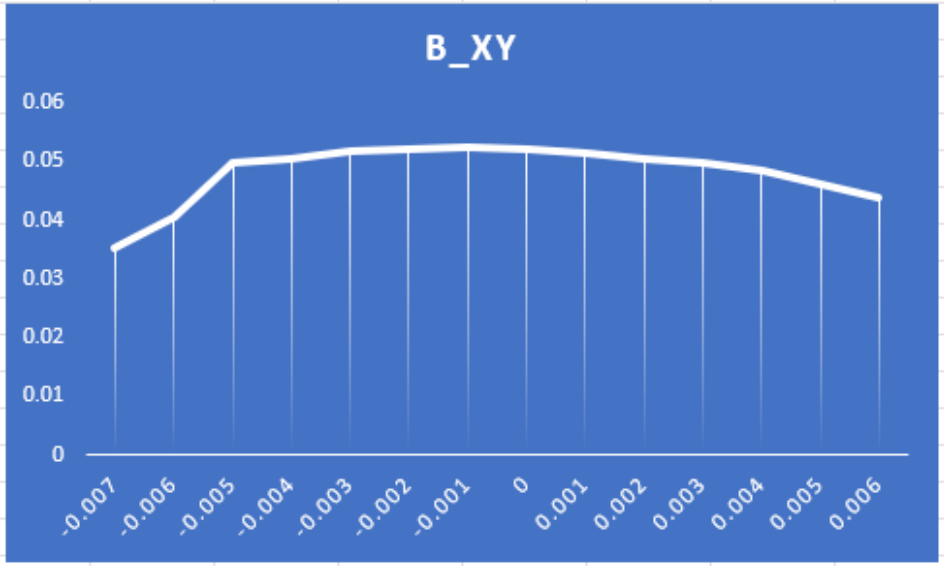
$$\beta_{ij} = \frac{3e^3\,\mathrm{sgn}(\mathcal{C})}{\pi h^2}\left[\frac{\nu_i^t \nu_j^t}{\nu_j^2}\frac{1}{\mathcal{W}_\mathcal{T}{}^2}\sum_{n=1}^{2}(-1)^n \sin(\gamma_n)\cos(\gamma_n)^3\right]$$

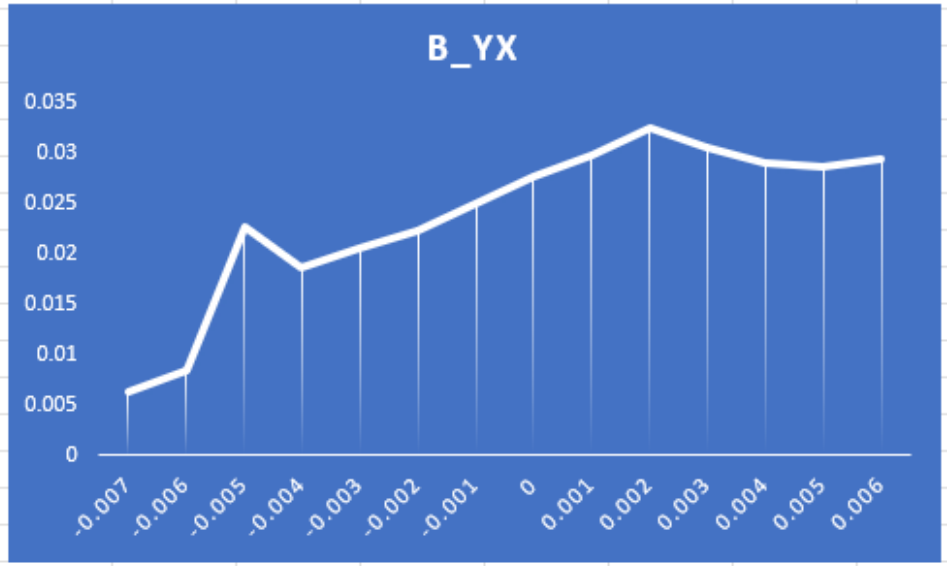
$$\gamma_n = \arcsin\{\frac{1}{\mathcal{W}_\mathcal{T}}[\frac{2|\mu|}{\hbar\omega} + (-1)^{n+1}]\}$$

Y

D=(b'-b)/b	-0.01	-0.009	-0.008	-0.007	-0.006	-0.005	-0.004	-0.003	-0.002	-0.001	0	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008
v^t_x				0.38894	0.42975	0.53614	0.51861	0.52045	0.51866	0.52175	0.51835	0.50821	0.50208	0.47762	0.45844	0.45123	0.4589		
v^t_y				0.67328	0.65691	0.53001	0.55525	0.5343	0.5193	0.49931	0.48185	0.46762	0.44922	0.45831	0.4645	0.45812	0.45079		
v^t_z				-0.7007	-0.6446	-0.4421	-0.4727	-0.4358	-0.4083	-0.3765	-0.3495	-0.3284	-0.3079	-0.3239	-0.339	-0.3473	-0.3569		
v_x				1.17568	1.03949	0.77863	0.81753	0.78682	0.766	0.73456	0.70348	0.67376	0.63892	0.65832	0.68289	0.7049	0.73742		
v_y				-0.4959	-0.4743	0.52611	0.49866	0.49783	0.50076	0.50796	0.51218	0.51285	0.51398	0.51559	0.52863	0.55522	0.6048		
v_z				0.68983	0.65637	0.59875	0.59665	0.58329	0.578	-0.5743	-0.5711	0.57011	0.56623	0.57716	0.59105	0.59337	0.6178		
d_x				-2.1869	2.82325	-0.246	2.72057	0.87795	0.23786	1.1082	1.26277	1.07789	0.94411	0.35876	0.59184	-1.2266	0.41581		
d_y				-4.9339	4.45259	-0.4205	-3.6924	-1.2932	-0.58	-1.1141	-1.331	-1.5124	-0.5201	-0.2974	-0.3459	3.03299	2.88029		
d_z				14.4251	-0.4774	-3.5505	-3.4279	-1.377	-0.4726	0.49627	0.92917	-1.6621	-0.9325	1.06901	3.45891	8.89094	12.0018		

D=b'-b	-0.01	-0.009	-0.008	-0.007	-0.006	-0.005	-0.004	-0.003	-0.002	-0.001	0	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008
B^t_xy				0.035222	0.040569	0.049817	0.050358	0.051573	0.052156	0.052446	0.052141	0.051495	0.050253	0.049826	0.048474	0.046189	0.043735		
B^t_yx				0.006266	0.008446	0.022744	0.018735	0.020646	0.02229	0.02508	0.027639	0.029836	0.032521	0.030563	0.029048	0.028656	0.029418		





Z																								
D=(b'-b)/b	-0.01	-0.009	-0.008	-0.007	-0.006	-0.005	-0.004	-0.003	-0.002	-0.001	0	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.01	0.011	0.012	
v^t_x	0.3694	0.3785	0.39343	0.41417	0.42919	0.44954	0.46427	0.47831	0.49249	0.50564	0.51809	0.53015	0.53611	0.54649	0.5512	0.56014	0.56262	0.5645	0.56627	0.56674	0.56751	0.560846	0.560878	
v^t_y	0.46345	0.46611	0.4685	0.4706	0.47281	0.47233	0.47438	0.4809	0.4759	0.48239	0.47947	0.4789	0.47855	0.48495	0.48686	0.48386	0.488	0.49433	0.49376	0.49763	0.49702	0.509419	0.508722	
v^t_z	-0.3691	-0.3679	-0.3669	-0.3662	-0.3644	-0.3608	-0.3583	-0.3633	-0.3504	-0.355	-0.3473	-0.3417	-0.3353	-0.3397	-0.3356	-0.328	-0.3297	-0.3337	-0.3282	-0.3304	-0.3255	-0.33888	-0.33452	
v_x	0.58044	0.59119	0.60499	0.62107	0.63387	0.64551	0.65701	0.68002	0.67561	0.69717	0.70073	0.70666	0.71109	0.73005	0.73673	0.73814	0.75232	0.76896	0.77166	0.78477	0.78701	0.81523	0.816837	
v_y	0.5558	0.54465	0.53983	0.53923	0.53475	0.53342	0.52901	0.52602	0.51982	0.51698	0.51108	0.50648	0.49844	0.49653	0.48994	0.48503	0.47904	0.47469	0.46759	0.4623	0.45571	0.450646	0.44442	
v_z	0.65892	0.64479	0.63158	0.6183	0.60794	0.59626	0.58897	0.58514	0.57603	0.57554	-0.5678	-0.5645	-0.5605	0.5647	0.564	0.56081	0.56144	0.56609	0.56265	0.56382	0.56062	0.567304	0.563469	
d_x	6.45243	3.43945	2.12391	2.6479	1.81544	1.77443	1.49279	1.79665	0.60637	1.53144	0.16523	0.19348	-1.4155	0.6561	0.49577	0.41973	0.1073	0.94567	0.31591	0.34	-0.1382	0.313212	-0.15218	
d_y	-3.3586	-1.1188	-0.3539	-1.1776	-0.8311	-0.6917	-0.8406	-1.4047	-0.4535	-1.5669	0.07706	0.04074	1.30296	-0.7895	-1.2468	-0.78	-0.4171	-1.4525	-1.0377	-0.8604	-0.539	-1.25745	-0.87658	
d_z	-4.3959	-2.6609	-2.017	-2.4533	-2.1442	-1.6873	-1.7317	-1.3969	-1.2723	-1.2536	-0.0741	-0.2176	-0.7218	0.23519	-0.5088	0.08153	0.72835	0.43927	0.27953	0.82118	0.62815	0.559498	0.403876	
D=b'-b	-0.01	-0.009	-0.008	-0.007	-0.006	-0.005	-0.004	-0.003	-0.002	-0.001	0	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009	0.01	0.011	0.012	
B^t_xy	0.038686	0.039998	0.041252	0.042497	0.043797	0.045047	0.046418	0.047819	0.049219	0.050693	0.052125	0.053588	0.055156	0.056562	0.058043	0.059447	0.060822	0.062028	0.063314	0.064369	0.06551	0.065882	0.066818	
B^t_yx	0.035471	0.033949	0.032845	0.032035	0.031171	0.030761	0.030094	0.028613	0.029138	0.027875	0.027728	0.027527	0.0271	0.026164	0.02567	0.025668	0.02466	0.023638	0.023248	0.022338	0.021964	0.020132	0.019779