

### Supporting information: Phase field crystal modeling of graphene/hexagonal boron nitride interfaces

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#### Model parameters for hexagonal crystals

Figure no.	$\epsilon_C$	$\epsilon_{BN}$	$\gamma_{C_{liquid}}$	$\gamma_{C_{solid}}$	$\gamma_{BN_{liquid}}$	$\gamma_{BN_{solid}}$	$\alpha_{B,C},$ $\alpha_{C,B}$	$\gamma_{B,C},$ $\gamma_{C,B}$	$\alpha_{N,C},$ $\alpha_{C,N}$	$\gamma_{N,C},$ $\gamma_{C,N}$	$\psi_{C_{liquid}}$	$\psi_{C_{solid}}$	$\psi_{BN_{liquid}}$	$\psi_{BN_{solid}}$
2	-0.15958	-0.111595	0.071834	-0.052149	-0.071122	0.053162	-0.12	0.0	-0.12	0.0	0.283274	0.252912	-0.419765	-0.291116
3	-0.228853	-0.334086	0.074632	-0.057991	-0.088174	0.052073	-0.12	0.0	-0.12	0.0	0.289753	0.251905	-0.517038	-0.374479

where  $\psi_{C_{liquid}}$  represents the average density of liquid state of graphene,  $\psi_{C_{solid}}$  is the average density of solid state of graphene,  $\psi_{BN_{liquid}}$  is the average density of liquid state of h-BN, and  $\psi_{BN_{solid}}$  represents the average density of solid state of h-BN.

#### Model parameters for truncated triangular crystals

Figure no.	$\epsilon_C$	$\epsilon_{BN}$	$\gamma_{C_{liquid}}$	$\gamma_{C_{solid}}$	$\gamma_{BN_{liquid}}$	$\gamma_{BN_{solid}}$	$\alpha_{B,C},$ $\alpha_{C,B}$	$\gamma_{B,C},$ $\gamma_{C,B}$	$\alpha_{N,C},$ $\alpha_{C,N}$	$\gamma_{N,C},$ $\gamma_{C,N}$	$\psi_{C_{liquid}}$	$\psi_{C_{solid}}$	$\psi_{BN_{liquid}}$	$\psi_{BN_{solid}}$
4	-0.223822	-0.186534	0.072398	-0.053071	-0.093665	0.049625	-0.183046	0.045753	-0.12	0.0	0.281774	0.259026	-0.464709	-0.354672
5	-0.223822	-0.186534	0.072398	-0.053071	-0.093665	0.049625	-0.12	0.0	-0.183046	0.045753	0.281774	0.259026	-0.464709	-0.354672
6	-0.230995	-0.256036	0.074792	-0.048257	-0.078683	0.043032	-0.157575	0.062894	-0.12	0.0	0.284558	0.255753	-0.474907	-0.414532
7	-0.230995	-0.256036	0.074792	-0.048257	-0.078683	0.043032	-0.12	0.0	-0.157575	0.062894	0.284558	0.255753	-0.474907	-0.414532

### Model parameters for truncated triangular crystals

8	-0.229479	-0.305749	0.074961	-0.041969	-0.092629	0.049282	-0.200349	0.052054	-0.12	0.0	0.287176	0.257963	-0.51293	-0.36216
9	-0.229479	-0.305749	0.074961	-0.041969	-0.092629	0.049282	-0.12	0.0	-0.200349	0.052054	0.287176	0.257963	-0.51293	-0.36216
10	-0.21496	-0.395893	0.086914	-0.053149	-0.081019	0.053994	-0.175488	0.077703	-0.12	0.0	0.299732	0.253086	-0.555927	-0.356388
11	-0.21496	-0.395893	0.086914	-0.053149	-0.081019	0.053994	-0.12	0.0	-0.175488	0.077703	0.299732	0.253086	-0.555927	-0.356388

### Model parameters for triangular crystals

Figure no.	$\epsilon_C$	$\epsilon_{BN}$	$\gamma_{C_{liquid}}$	$\gamma_{C_{solid}}$	$\gamma_{BN_{liquid}}$	$\gamma_{BN_{solid}}$	$\alpha_{B,C}, \alpha_{C,B}$	$\gamma_{B,C}, \gamma_{C,B}$	$\alpha_{N,C}, \alpha_{C,N}$	$\gamma_{N,C}, \gamma_{C,N}$	$\psi_{C_{liquid}}$	$\psi_{C_{solid}}$	$\psi_{BN_{liquid}}$	$\psi_{BN_{solid}}$
12	-0.167022	-0.547672	0.076349	-0.056206	-0.073079	0.044255	-0.249428	0.038286	-0.12	0.0	0.296878	0.252925	-0.616218	-0.383265
13	-0.167022	-0.547672	0.076349	-0.056206	-0.073079	0.044255	-0.12	0.0	-0.249428	0.038286	0.296878	0.252925	-0.616218	-0.383265
14	-0.224973	-0.402736	0.083795	-0.040526	-0.098198	0.052531	-0.209042	0.071671	-0.12	0.0	0.292715	0.254977	-0.538943	-0.378668
15	-0.224973	-0.402736	0.083795	-0.040526	-0.098198	0.052531	-0.12	0.0	-0.209042	0.071671	0.292715	0.254977	-0.538943	-0.378668
16	-0.216859	-0.352195	0.073594	-0.059287	-0.098732	0.048703	-0.266971	0.041044	-0.12	0.0	0.280079	0.256785	-0.548182	-0.356935
17	-0.216859	-0.352195	0.073594	-0.059287	-0.098732	0.048703	-0.12	0.0	-0.266971	0.041044	0.280079	0.256785	-0.548182	-0.356935

### Model parameters for triangular jagged crystals

Figure no.	$\epsilon_C$	$\epsilon_{BN}$	$\gamma_{C_{liquid}}$	$\gamma_{C_{solid}}$	$\gamma_{BN_{liquid}}$	$\gamma_{BN_{solid}}$	$\alpha_{B,C},$ $\alpha_{C,B}$	$\gamma_{B,C},$ $\gamma_{C,B}$	$\alpha_{N,C},$ $\alpha_{C,N}$	$\gamma_{N,C},$ $\gamma_{C,N}$	$\psi_{C_{liquid}}$	$\psi_{C_{solid}}$	$\psi_{BN_{liquid}}$	$\psi_{BN_{solid}}$
18	-0.196965	-0.29042	0.072597	-0.044556	-0.070802	0.057816	-0.22925	0.037588	-0.12	0.0	0.282786	0.251068	-0.489828	-0.435001
19	-0.196965	-0.29042	0.072597	-0.044556	-0.070802	0.057816	-0.12	0.0	-0.22925	0.037588	0.282786	0.251068	-0.489828	-0.435001

### Model parameters for supporting information

#### Contents

1. Hexagonal h-BN crystals with single and multiple layers
2. Multilayer jagged triangular crystals

### Model parameters for hexagonal h-BN crystals with single and multiple layers

Figure no.	$\epsilon_C$	$\epsilon_{BN}$	$\gamma_{C_{liquid}}$	$\gamma_{C_{solid}}$	$\gamma_{BN_{liquid}}$	$\gamma_{BN_{solid}}$	$\alpha_{B,C},$ $\alpha_{C,B}$	$\gamma_{B,C},$ $\gamma_{C,B}$	$\alpha_{N,C},$ $\alpha_{C,N}$	$\gamma_{N,C},$ $\gamma_{C,N}$	$\psi_{C_{liquid}}$	$\psi_{C_{solid}}$	$\psi_{BN_{liquid}}$	$\psi_{BN_{solid}}$
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**Model parameters for hexagonal h-BN crystals with single and multiple layers**

S.1	-0.163363	-0.282096	0.070165	-0.047456	-0.085766	0.048946	-0.12	0.0	-0.12	0.0	0.294354	0.255123	-0.496608	-0.358141
S.2	-0.19347	-0.348853	0.079408	-0.056102	-0.072194	0.0559	-0.12	0.0	-0.12	0.0	0.299478	0.255731	-0.507775	-0.309232
S.3	-0.234486	-0.303063	0.087854	-0.049232	-0.082104	0.04629	-0.12	0.0	-0.12	0.0	0.281286	0.255009	-0.488791	-0.316017
S.4	-0.196595	-0.262365	0.070668	-0.056781	-0.080145	0.042274	-0.12	0.0	-0.12	0.0	0.284627	0.246777	-0.462841	-0.430125
S.5	-0.192275	-0.311261	0.073331	-0.049879	-0.071732	0.058537	-0.12	0.0	-0.12	0.0	0.288787	0.249603	-0.485752	-0.362487
S.6	-0.163992	-0.350473	0.081059	-0.042846	-0.077607	0.047931	-0.12	0.0	-0.12	0.0	0.291355	0.247824	-0.492146	-0.414443
S.7	-0.216684	-0.353494	0.08855	-0.059164	-0.086036	0.052253	-0.12	0.0	-0.12	0.0	0.284885	0.24748	-0.495003	-0.357658
S.8	-0.156623	-0.368561	0.083114	-0.051556	-0.075749	0.055546	-0.12	0.0	-0.12	0.0	0.290814	0.254076	-0.51875	-0.362763
S.9	-0.198403	-0.276812	0.071228	-0.053221	-0.070372	0.045822	-0.12	0.0	-0.12	0.0	0.290819	0.257861	-0.475742	-0.364005
S.10	-0.229859	-0.233182	0.082978	-0.053568	-0.071177	0.044479	-0.12	0.0	-0.12	0.0	0.282413	0.255706	-0.472612	-0.360508
S.11	-0.178794	-0.399035	0.089572	-0.045836	-0.081847	0.051427	-0.12	0.0	-0.12	0.0	0.285779	0.246865	-0.516831	-0.384876
S.12	-0.238818	-0.422435	0.085332	-0.043547	-0.07481	0.05809	-0.12	0.0	-0.12	0.0	0.287313	0.247261	-0.546598	-0.367689
S.13	-0.193625	-0.382327	0.07839	-0.051031	-0.085808	0.041175	-0.12	0.0	-0.12	0.0	0.285476	0.258271	-0.536733	-0.34035

**Model parameters for multilayer jagged triangular crystals**

### Model parameters for multilayer jagged triangular crystals

Figure no.	$\epsilon_C$	$\epsilon_{BN}$	$\gamma_{C_{liquid}}$	$\gamma_{C_{solid}}$	$\gamma_{BN_{liquid}}$	$\gamma_{BN_{solid}}$	$\alpha_{B,C},$ $\alpha_{C,B}$	$\gamma_{B,C},$ $\gamma_{C,B}$	$\alpha_{N,C},$ $\alpha_{C,N}$	$\gamma_{N,C},$ $\gamma_{C,N}$	$\psi_{C_{liquid}}$	$\psi_{C_{solid}}$	$\psi_{BN_{liquid}}$	$\psi_{BN_{solid}}$
S.2.1	-0.197327	-0.39235	0.071516	-0.049434	-0.081975	0.058222	-0.192917	0.077268	-0.12	0.0	0.291139	0.255959	-0.523378	-0.42061
S.2.2	-0.197327	-0.39235	0.071516	-0.049434	-0.081975	0.058222	-0.12	0.0	-0.192917	0.077268	0.291139	0.255959	-0.523378	-0.42061
S.2.3	-0.171664	-0.385224	0.075096	-0.044481	-0.083357	0.056888	-0.244712	0.099279	-0.12	0.0	0.285781	0.255077	-0.540368	-0.356119
S.2.4	-0.171664	-0.385224	0.075096	-0.044481	-0.083357	0.056888	-0.12	0.0	-0.244712	0.099279	0.285781	0.255077	-0.540368	-0.356119
S.2.5	-0.234192	-0.329991	0.075243	-0.044407	-0.095656	0.047296	-0.209936	0.043544	-0.12	0.0	0.284464	0.253543	-0.503632	-0.321436
S.2.6	-0.234192	-0.329991	0.075243	-0.044407	-0.095656	0.047296	-0.12	0.0	-0.209936	0.043544	0.284464	0.253543	-0.503632	-0.321436