III-V Semiconductors which can be described by Tersoff potential

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Tersoff potential The potential used in the study is developed by Tersoff:

$$E = \frac{1}{2}\sum_i \sum_{j \neq i} V_{ij}$$

$$V_{ij} = f_C(r_{ij})[f_R(r_{ij}) + b_{ij} f_A(r_{ij})]$$

$$f_C(r_{ij}) = \begin{cases} 1 & r_{ij} < R_{ij}(R-D), \\ \frac{1}{2} + \frac{1}{2}cos(\pi \frac{r_{ij}-R_{ij}}{S-ij-R_{ij}})(\frac{1}{2} + \frac{1}{2}cos(\pi \frac{r-R}{D})) & R_{ij}(R-D) < r_{ij} < S_{ij}(R+D), \\ 0 & r_{ij} > S_{ij}(R+D) \end{cases}$$

$$f_R(r) = Aexp(-\lambda_1 r)$$

$$f_A(r) = -Bexp(-\lambda_2 r)$$

$$b_{ij} = \frac{\chi_{ij}}{(1+\beta^n \zeta_{ij}^n)^{1/2n}}$$

$$\zeta_{ij} = \sum_{k \neq i,j} f_C(r_{ij}) g(\theta_{ijk}) exp(\lambda_3^3 (r_{ij} - r_{ik})^3)$$

$$g(\theta) = 1 + \frac{c^2}{d^2} - \frac{c^2}{[d^2 + (h - cos(\theta))^2]}$$

III-V Semiconductors parameters I will give a table of parameters of the following materials(1,2,3,1,2).

- BN,CBN(https://doi.org/10.1103/PhysRevB.86.115410)
- BP(https://doi.org/10.1016/S0378-4371(02)00780-X)
- BAs(https://doi.org/10.1016/S0375-9601(99)80004-8)

- AIN(https://doi.org/10.1016/j.chemphys.2004.03.030)
- InGaAs, InAlAs and GaAsSb (http://iopscience.iop.org/article/10.1088/0268-1242/28/8/085011/meta))
- GaN(https://doi.org/10.1016/S0375-9601(03)01039-9))
- amorphous silicon nitride(https://doi.org/10.1103/PhysRevB.58.8323)
- GeC and GeSi (https://doi.org/10.1088/1367-2630/4/1/309)

	Si-C	Ge-c	Al-Al	Al-N	N-N
A(eV)	1597.31	1570.12	746.698	3000.214	636.814
B(eV)	404.17	381.24	40.451	298.81	511.76
λ_1	2.98390	2.9665	2.4647	3.53051	5.43673
λ_2	1.97205	1.9583	0.9683	1.99995	2.7
λ_3	1	1	1	1	1
β	6.2862×10^{-7}	5.2945×10^{-7}	1.094932	1.1566×10^{-4}	5.2938×10^{-3}
n	0.757425	0.74189	6.085605	1.33041	1.33041
c	69219.5	72239.5	0.074836	2.0312×10^{4}	2.0312×10^{4}
d	10.3005	10.018	19.569127	16.5103	20.312
h	-0.584415	-0.50471	-0.659266	-0.58239	-0.56239
R($10^{-10}m$)	2.33	2.41	3.4	2.335	1.8
D($10^{-10}m$)	0.15	0.15	0.2	0.15	0.2
χ	0.97	0.94	1	1	1

Table 1: SiC,GeC and AlN

	B-P	B-As	Ga-Ga	Ga-N	N-N
A(eV)	2633.3	3469.00	2839.82	3732.08	11000
B(eV)	325.11	320.00	114.786	234.013	219.45
λ_1	3.4207	3.10	3.2834	3.6987	5.7708
λ_2	1.898	1.6	1.7154	1.9214	2.5115
λ_3	1	1	1	1	1
β	1.59365×10^{-4}	1.10×10^{-6}	2.3586×10^{-1}	1.0900×10^{-6}	1.0562×10^{-1}
n	0.766	0.72	3.47290	0.78734	12.4498
c	1.0021×10^{5}	1.00390×10^{5}	7.6298×10^{-2}	7.2239	7.9934×10^{4}
d	16.7601	16.217	19.796	10.018	134.32
h	-0.6281	-0.59825	7.1559	-0.5180	-0.9973
R($10^{-10}m$)	2.5	2.395	2.8	2.4	2.0
D(S)($10^{-10}m$)	0.2	0.15	3.0	2.6	2.3
χ	1	1	1	1	1

Table 2: BP and GaN

And we can give two parameter figure of CBN and InGaAs, InAlAs and GaAsSb:

	Si-N	Si-Si	Ga-N	N-N	In-As
A(eV)	6368.14	1830.8	3732.08	11000	2291.292969
B(eV)	511.76	471.18	234.013	219.45	424.874512
λ_1	5.43673	2.4799	3.6987	5.7708	2.517917
λ_2	2.70000	1.7322	1.9214	2.5115	1.678611
λ_3	1	12	1	1	1.5
β	5.29380×10^{-3}	1.1000×10^{-6}	1.0900×10^{-6}	1.0562×10^{-1}	0.3779
n	1.33041	0.78734	0.78734	12.4498	7.141472
c	2.03120×10^{4}	1.0039×10^{5}	7.2239	7.9934×10^{4}	0.9989
d	25.5103	16.217	10.018	134.32	0.82608
h	-0.56239	-0.59825	-0.5180	-0.9973	-0.5145
R($10^{-10}m$)	1.80	2.70	2.4	2.0	3.6
S($10^{-10}m$)	2.10	3.00	2.6	2.3	3.8
χ	0.65	0.65	1	1	

Table 3: Si_3N_4 and GaN

Parameters	C B *X*	C C *X*	C N *X*	B C *X*	B N *X*	N B *X*	N C *X*
A (eV)	1386.78	1393.6	1386.78	1386.78	1380.0	1380.0	1386.78
$B^{'}$ (eV)	339.068 91	430.0	387.575 15 2	339.068 91 0	340.0	340.0	387.575 15 2
λ^{I} (Å^{-1})	3.5279	3.4879	3.5279	3.5279	3.568	3.568	3.5279
λ^{II} (Å^{-1})	2.2054	2.2119	2.2054	2.2054	2.199	2.199	2.2054
n	0.727 51	0.727 51	0.727 51	0.727 51	0.727 51	0.727 51	0.727 51
β (10^{-7})	1.5724	1.5724	1.5724	1.257 24	1.257 24	1.257 24	1.257 24
c	38 049	38 049	38 049	25 000	25 000	25 000	25 000
d	4.3484	4.3484	4.3484	4.3484	4.3484	4.3484	4.3484
h	−0.93	−0.93	−0.93	−0.89	−0.89	−0.89	−0.89
R (Å)	1.85	1.80	1.85	1.85	1.90	1.90	1.85
S (Å)	2.05	2.10	2.05	2.05	2.00	2.00	2.05

Figure 1: The parameters of the Terso potential optimized for C-BN interactions. The atom X represents the bond-modifying element where all parameters are exactly the same whether it is C, B, or N

Parameter	GaAs Powell [27]	AlAs Powell [26]	GaSb Powell [27]	
D_e	2.126 73	2.3347	2.170 13	
S	1.602 28	1.541 31	1.412 56	
r_e	2.352 18	2.368 43	2.485 49	
β	1.562 95	1.448 45	1.477 05	
γ	0.363 585	0.359 702	0.369 53	
n	5.436 47	8.369 92	4.616 25	
c	1.205 95	1.050 25	1.179 45	
d	0.800 338	0.850 097	0.842 774	
h	−0.442 817	−0.458 041	−0.429 907	
λ	1.830 57	1.384 02	1.8244	
Parameter	InAs Powell [27]	InAs Migliorato [22]	InAs Titantah [23]	InAs Adhikari [24]
D_e	2.131 23	2.1643	1.729 05	5.172 83
S	1.470 58	1.5	1.246 46	1.826 12
r_e	2.499 36	2.4908	2.577 05	2.213 81
β	1.498 07	1.453 72	1.475 71	1.3592
γ	0.379 62	0.3779	0.0053	0.318 64
n	7.038 76	7.141 47	0.83	0.756 169
c	1.009 04	0.9989	0.8495	5.172 42
d	0.823 55	0.826 08	0.4	1.665 97
h	−0.462 05	−0.5145	−0.254	−0.541 33
λ	1.4331	1.5	2.33	2.597 56

Figure 2: This table lists all input parameter sets for modeling $In_xGa_{1-x}As, In_xAl_{1-x}AsandGaAs_{1-x}Sb_x$ interactions, using the empirical Terso potential.