Tight binding analysis of Si and GaAs ultra thin bodies with subatomic resolution

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I. PARAMETERS OF UNSTRAINED GAAS

Tight Binding model	sp3d5s*
Interaction range	First nearest neighbour (4 neighbours per atom)
Target bands	Hybrid functional calculations (HSE06) by VASP(v 5.2.3)
Date obtained	Aug 2014
Reference	Y. Tan,et al http://arxiv.org/abs/1503.04781 (2015)
Authors	Yaohua P. Tan
Nemo5 Database	param_HSE06_mapping

TABLE I: Description of the parameters

sp3d5s* Tight Binding parameters of Si are given by table II. The band structure and DOS of GaAs are shown in 1 respectively. The effective masses and important bandedges are compared in table III.

GaAs			
a_0	5.6307Å		
E_{s_a}	−8.063758	E_{s_c}	−1.603222
E_{p_a}	3.126841	E_{p_c}	4.745896
$E_{s_a^*}$	21.930865	$E_{s_c^*}$	23.630466
E_{d_a}	13.140998	E_{d_c}	14.807586
Δ_a	0.194174	Δ_c	0.036594
$V_{s_a s_c \sigma}$	−1.798514		
$V_{s_a^* s_c^* \sigma}$	−4.112848		
$V_{s_a s_c^* \sigma}$	−1.258382	$V_{s_c s_a^* \sigma}$	−1.688128
$V_{s_a p_c \sigma}$	3.116745	$V_{s_c p_a \sigma}$	2.776805
$V_{s_a^* p_c \sigma}$	1.635158	$V_{s_c^* p_a \sigma}$	3.381868
$V_{s_a d_c \sigma}$	−0.396407	$V_{s_c d_a \sigma}$	−2.151852
$V_{s_a^* d_c \sigma}$	−0.145161	$V_{s_c^* d_a \sigma}$	−0.810997
$V_{p_a p_c \sigma}$	4.034685		
$V_{p_a p_c \pi}$	−1.275446		
$V_{p_a d_c \sigma}$	−1.478036	$V_{p_c d_a \sigma}$	−0.064809
$V_{p_a d_c \pi}$	1.830852	$V_{p_c d_a \pi}$	2.829426
$V_{d_a d_c \sigma}$	−1.216390		
$V_{d_a d_c \pi}$	2.042009		
$V_{d_a d_c \delta}$	−1.829113		

TABLE II: Slater Koster type ETB parameters of bulk GaAs. All presented parameters except for the lattice constants are in the unit of eV. The lattice constants are in Angstrom.

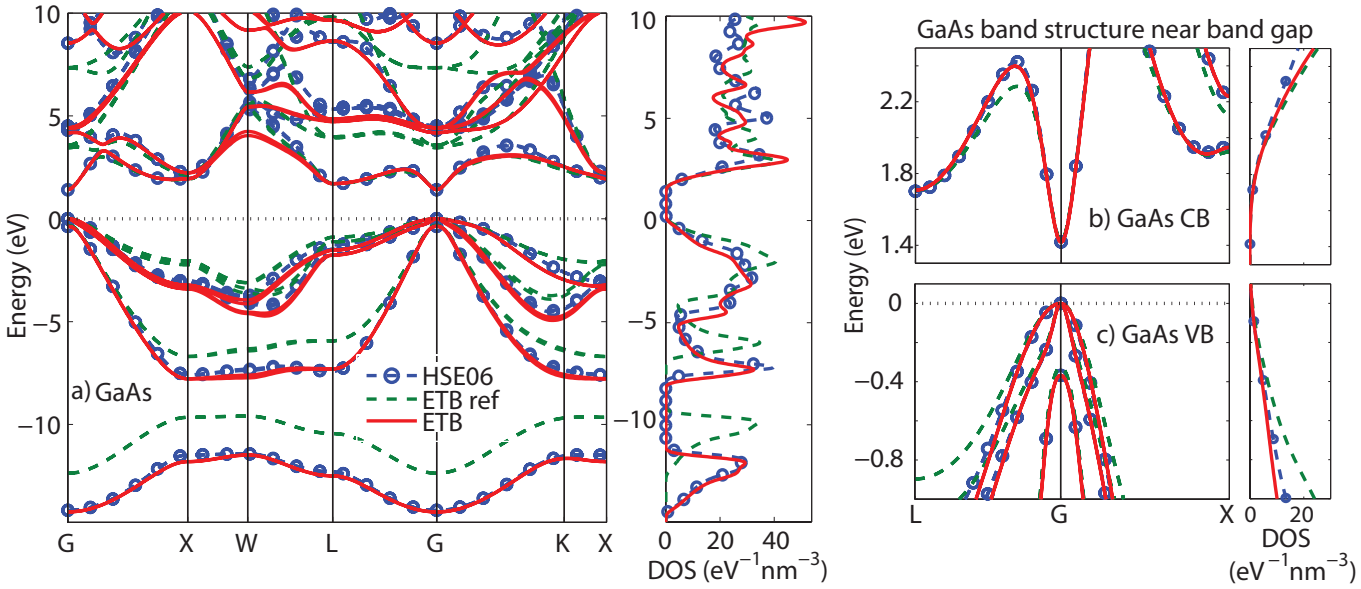

FIG. 1: Band structure and density of states of bulk GaAs. ETB band structure agree with the HSE06 band structure (a), especially for bottom conduction bands (b) and top valence bands(c).

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	GaAs			
targets	TB Ref	HSE06	TB	error(%)
$E_g(\Gamma)$	1.424	1.418	1.416	0.2
$E_g(X)$	1.900	1.919	1.910	0.5
$E_g(L)$	1.707	1.702	1.708	0.3
Δ_{SO}	0.326	0.368	0.367	0.1
m_{hh100}	0.383	0.310	0.337	8.510
m_{hh110}	0.667	0.573	0.619	7.879
m_{hh111}	0.853	0.750	0.813	8.507
m_{lh100}	0.085	0.082	0.083	0.744
m_{lh110}	0.078	0.073	0.074	1.614
m_{lh111}	0.076	0.071	0.072	1.715
m_{so100}	0.166	0.164	0.160	1.998
m_{so110}	0.166	0.164	0.160	2.037
m_{so111}	0.166	0.164	0.160	2.041
m_{c100}	0.068	0.065	0.067	2.787
m_{c110}	0.068	0.066	0.067	2.790
m_{c111}	0.068	0.065	0.067	2.781
m_{cXl}	1.526	1.577	1.480	6.142
m_{cXt}	0.177	0.215	0.204	5.083
m_{cLl}	1.743	1.626	1.446	11.055
m_{cLt}	0.099	0.111	0.136	22.614

TABLE III: Targets comparison of bulk GaAs. Critical band edges and effective masses at Γ, X and L from TB and HSE06 calculations are compared. The E_g and Δ_{SO} are in the unit of eV; effective masses are scaled by free electron mass m_0. The error column summarizes the discrepancies between HSE06 and TB results.