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

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I. PARAMETERS OF UNSTRAINED ALAS

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	
Authors	Yaohua P. Tan
Nemo5 Database	

TABLE I: Description of the parameters

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

AlAs	
a_0	5.6307$\mathring{A}$
E_{s_c}	3.844665
E_{p_c}	9.171503
E_{s*_c}	27.975218
E_{d_c}	16.991734
λ_c	0.000000
E_{s_a}	−2.932564
E_{p_a}	7.882933
E_{s*_a}	27.897857
E_{d_a}	16.219579
λ_a	0.220931
$V_{s_c s_a \sigma}$	−1.884234
$V_{s*_c s*_a \sigma}$	−4.385365
$V_{s_c s*_a \sigma}$	−1.968153
$V_{s_c p_a \sigma}$	2.767410
$V_{s*_c p_a \sigma}$	2.568816
$V_{s_c d_a \sigma}$	−2.332389
$V_{s*_c d_a \sigma}$	−0.407474
$V_{p_c p_a \sigma}$	4.440040
$V_{p_c p_a \pi}$	−1.320667
$V_{p_c d_a \sigma}$	−1.373361
$V_{p_c d_a \pi}$	2.128562
$V_{d_c d_a \sigma}$	−1.406632
$V_{d_c d_a \pi}$	2.043294
$V_{d_c d_a \delta}$	−1.649027
$V_{s_a s_c \sigma}$	−1.884234
$V_{s*_a s*_c \sigma}$	−4.385365
$V_{s_a s*_c \sigma}$	−1.264778
$V_{s_a p_c \sigma}$	3.342574
$V_{s*_a p_c \sigma}$	2.386662
$V_{s_a d_c \sigma}$	−1.776396
$V_{s*_a d_c \sigma}$	−0.879660
$V_{p_a p_c \sigma}$	4.440040
$V_{p_a p_c \pi}$	−1.320667
$V_{p_a d_c \sigma}$	−1.141253
$V_{p_a d_c \pi}$	2.314171
$V_{d_a d_c \sigma}$	−1.406632
$V_{d_a d_c \pi}$	2.043294
$V_{d_a d_c \delta}$	−1.649027

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

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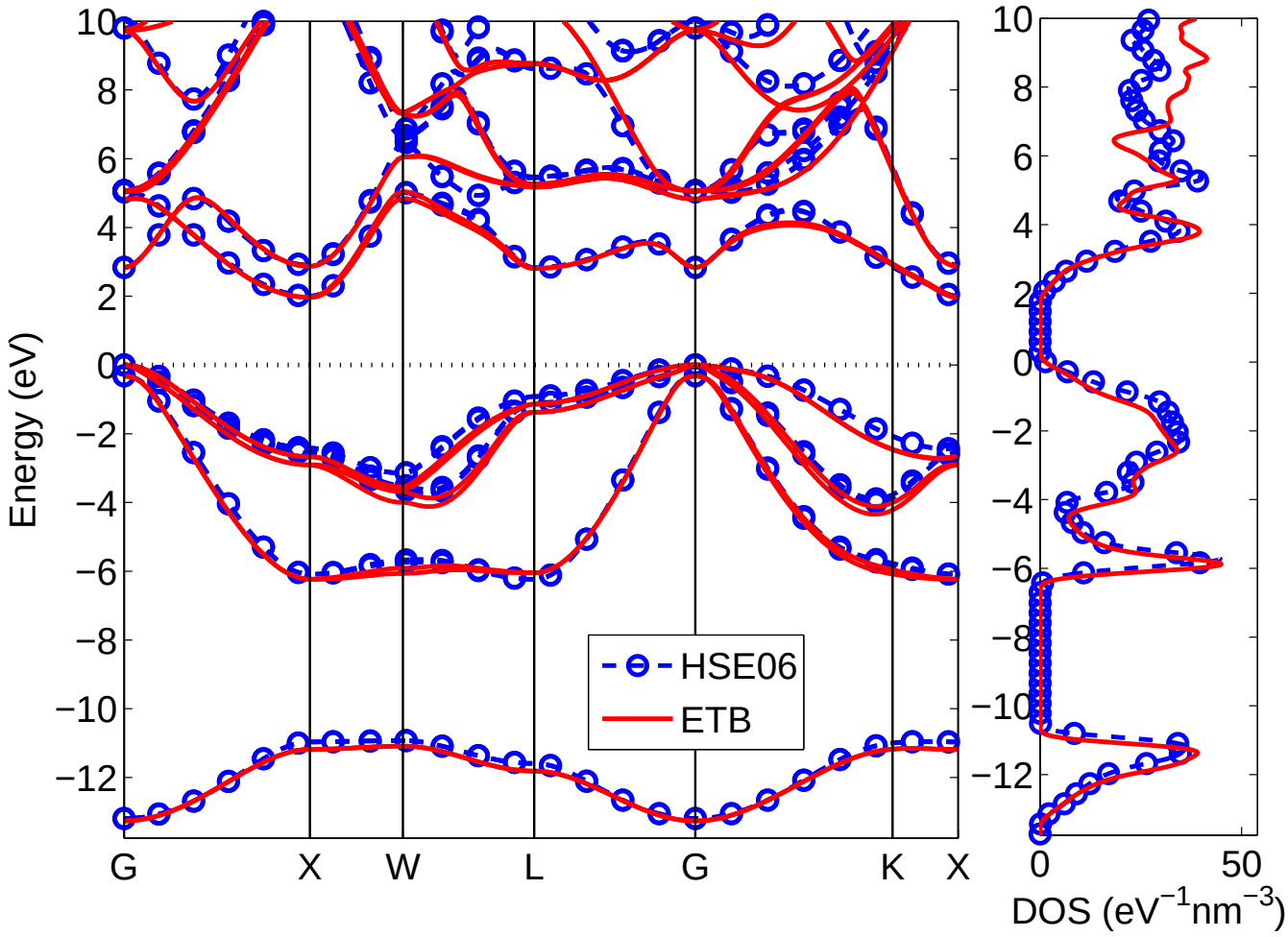

FIG. 1: Band structure and density of states of bulk AlAs. ETB band structure agree with the HSE06 band structure (a), especially for bottom conduction bands (b) and top valence bands(c).

Target	DFT (eV)	TB (eV)	error(%)
$E_g(\Gamma)$	4.186400	4.185930	0.0
$E_g(X)$	2.272698	2.261840	0.5
$E_g(L)$	3.632959	3.602002	0.9
$Delta_{SO}$	0.064749	0.061687	4.7
$E_v(\Gamma)$	4.080850	4.132198	1.3
γ_1	2.831	3.000	5.963
γ_2	0.548	0.586	6.997
γ_3	0.931	0.991	6.438
m_{hh100}	0.508	0.482	5.151
m_{hh110}	0.998	0.944	5.358
m_{hh111}	1.273	1.224	3.812
m_{lh100}	0.250	0.235	5.967
m_{lh110}	0.201	0.190	5.686
m_{lh111}	0.193	0.181	5.885
m_{so100}	0.343	0.319	6.881
m_{so110}	0.343	0.320	6.839
m_{so111}	0.343	0.320	6.895
m_{c100}	0.189	0.190	0.297
m_{c110}	0.189	0.190	0.285
m_{c111}	0.189	0.190	0.278
m_{cXL}	0.781	0.742	4.910
m_{cXT}	0.242	0.215	11.401
m_{cLL}	1.610	1.641	1.924
m_{cLT}	0.177	0.179	0.758
m_{c2XT}	0.236	0.251	6.484

TABLE III: Targets comparison of bulk AlAs. 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.