Modeling Alternative High Dielectric Constant Thin Films

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The Search for Alternative Dielectric Materials

- Application: Gate Dielectric in Transistors and Memory Applications
- Conventional Dielectric SiO₂ (Dielectric Constant $\kappa=3.9$)
- Thinner dielectric layer $\Rightarrow$ smaller, faster transistors

Fig. 1: Typical transistor configuration
Project Focus

- Create unit cell models of dielectric crystal structures using WIEN2K software
- Study simulated band structures to find band gaps, band offsets
- Unit cell models will provide foundation for future work
Starting WIEN2K

- Define unit cell parameters
- Initialization

Fig. 2: Ta$_2$O$_5$ unit cell.

Fig. 3: The graphical user interface for WIEN2K, w2web.
WIEN2K: Big Number Crunching

- Software minimizes energy of the crystal according to density functional theory and iterates until orbital equations are self-consistent.
- I used generalized gradient approximation (GGA) for exchange correlation energies.
- Linearized augmented plane wave (LAPW) method solves orbital equations.
WIEN2K: Simulated Measurements

- Band structure most important

Fig. 4: Band structure of Ge.


Valence bands: 4p, 4s, some 3d

Conduction bands

Band gap

Wavevector symmetry directions
Results
Fig. 5: alpha-quartz crystal structure.

Alpha-quartz (SiO$_2$)

- Looks like an insulator
- Band gap (6 eV) underestimated by local spin-density approximation (LSDA)
- Actual band gap: 8.9 eV

Fig. 6: Simulated band structure of alpha-quartz.

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Fig. 7: alpha-\(\text{Al}_2\text{O}_3\) crystal structure.

Alpha-\(\text{Al}_2\text{O}_3\)

- Alternative dielectric material
- Smaller underestimation
- 6.3 eV (graph) vs. 6.7 eV (literature)
- \(\kappa = 9\)

Fig. 8: Simulated band structure of \(\text{Al}_2\text{O}_3\).
Fig. 9: beta-cristobalite crystal structure.

Another structural possibility for SiO$_2$ in future models

Conduction bands appear shifted down

Band gap = 6 eV (compared to 8 eV in literature sources)

Fig. 10: Beta-cristobalite simulated band structure graph.

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Fig. 11: monoclinic HfO$_2$ crystal structure.

HfO₂

- Not studied as much
- HfO₂ model band gap = 4.2 eV
- Uncertainty in literature sources: 5.0 to 6.0 eV
- Model suggests gap is toward the lower end of that range
- $\kappa = 25$

Fig. 12: Simulated HfO₂ band structure
Fig. 13: Silicon crystal structure (clathrate).

Silicon

- Band gap is about 50% of what it should be (0.5 vs. 1.1 eV)
- Shape of lines is correct, however

Fig. 14: Simulated silicon band structure
Summary - Conclusions

- WIEN2K simulated band structures are accurately shaped
- Band gap generally underestimated by 25 to 33%
- Band offsets could not be extracted from band structure graphs
Improving Accuracy

- Underestimation due to excited conduction bands
- Including spin-orbit interactions could give a better representation of electron energy

\[ V_a(r) = V_0 \frac{r_0}{r} \exp\left[-\left(\frac{r}{r_0}\right)^2\right] \]
Future Work

- Build supercells with vacancies included
- Model dielectric/Si interface
- Experiments with alternative dielectric thin films

Fig. 15: Electron micrograph of HfO₂/Si interface.

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