Modeling Electron Energy-Loss Spectra of Dislocations in Silicon and Diamond

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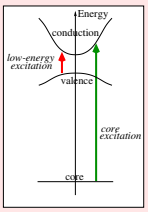
Summary

Dislocations in semiconductors can strongly influence the electrical and optical properties. Electron energy-loss spectroscopy (EELS) performed near dislocation cores is one of the few experimental techniques that can yield information about the electronic levels associated with dislocations, both within and above the band gap. Recent EELS spectra measured near dislocations in Si and diamond have shown differences from bulk regions [1, 2], but there are still issues regarding their interpretation.

Here, using ab initio calculations, we model and predict EELS spectra acquired on dislocation cores of various partial dislocations in silicon and diamond, and compare the results with bulk spectra. In particular, we consider various core structures of the 30°, 60°, & 90° glide and shuffle dislocations. In diamond, we find evidence of empty states localised on shuffle cores below the bulk band edge. In silicon, we find changes—analogue to those seen experimentally—in core-excitation EELS spectra near stacking faults and partial glide dislocations. This information could prove crucial to help resolve whether any electrical or optical activity is associated with undecorated dislocations in these materials.

What is EELS?

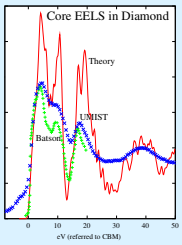
- Electron Energy Loss Spectroscopy
  - measure change in energy E of primary e^- as they induce secondary electronic transitions in a thin sample



- Low-loss EELS spectroscopy (0–20 eV): valence to conduction band transitions, provides an indirect measure of the dielectric function $\varepsilon(E)$, as the signal obtained is proportional to $\mathrm{Im}(-1/\varepsilon(E))$,
- Excitation from core level (ELNES: Energy Loss Near Edge Structure)

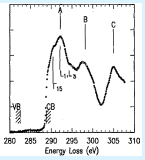
Bulk diamond

- Core EELS of bulk diamond: comparison with two experimental results: on type IIb diamond [2], and on diamond nanocrystals [3]
- Absorption in the gap may be attributed primarily to nanocrystal surface effects

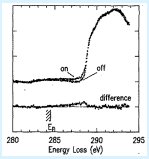


Experimental data on dislocations

- Diamond: type-IIb [2]



Bulk diamond



On/off dislocation

- Silicon: [1]

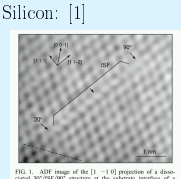


FIG. 1. ADF image of the [1 −1 0] projection of a dissociated 30°/ISF/90° structure at the substrate interface of a strained Si quantum well. The Si interface is indicated by the dashed line.

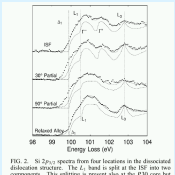
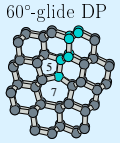


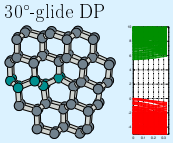
FIG. 2. Si $2p_{3/2}$ spectra from four locations in the dissociated dislocation structure. The L_3 band is split at the ISF into two components. This splitting is present also at the P30 core but not at P90. Both dislocation cores support recombination-edge gap states at L_3, but the ISF does not.

Diamond dislocations: Glide set

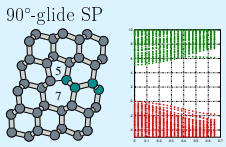
60°-glide DP



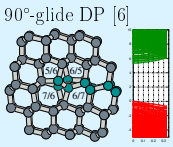
30°-glide DP



90°-glide SP



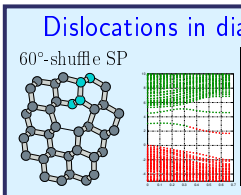
90°-glide DP [6]



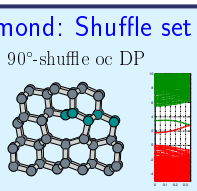
- No levels below the conduction band minimum (CBM) for reconstructed glide dislocations with four-fold coordinated atoms in the core

Dislocations in diamond: Shuffle set

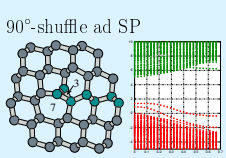
60°-shuffle SP



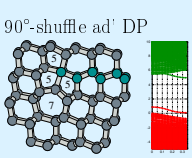
90°-shuffle oc DP



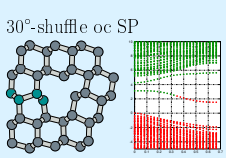
90°-shuffle ad SP



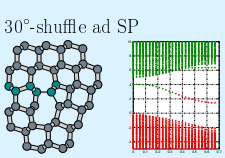
90°-shuffle ad' DP



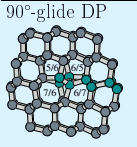
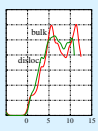
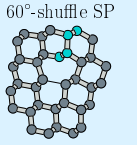
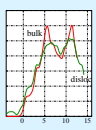
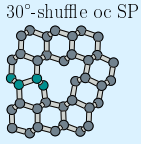
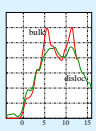
30°-shuffle oc SP



30°-shuffle ad SP



EELS on diamond dislocations

Structure	*Low-loss EELS*	*Core EELS*
90°-glide DP		
60°-shuffle SP		
30°-shuffle oc SP		

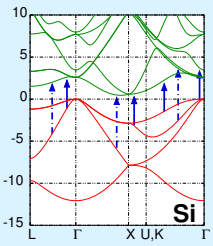
Relative core energies

Using scc-DFTB, we estimate relative core energies of dislocations in diamond (in eV/Å):

60° dislocations		90° partials		30° partials	
glide	0.0	glide DP	0.00	glide	0.0
shuffle	+0.5	glide SP	+0.17	shuffle oc	+1.2
		shuffle oc	+0.55	shuffle ad	+2.2

Methodology

- Self-consistent *ab initio* DFT calculations with AIMPRO code [4]
- Atom-centered s, p, d-like Gaussian orbitals
- BHS pseudopotentials



- Initial relaxation of dislocation cores using the self-consistent charge density functional tight-binding method (scc-DFTB) [5]
- For low-energy EELS, sum matrix elements over bands:

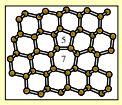
$$\varepsilon_2(\omega) = \frac{4\pi e^2}{\Omega} \sum_{n,\mathbf{k}} |\langle \Psi^n_{\mathbf{k}} | \mathbf{r} | \Psi^i_{\mathbf{k}} \rangle|^2 \delta(E^n_{\mathbf{k}} - E^i_{\mathbf{k}} - \hbar\omega) \qquad (1)$$

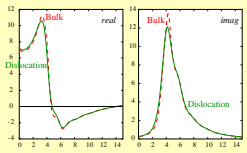
- For core-EELS, we compute the partial density of states, decomposed into suitable angular momenta around the atoms of interest

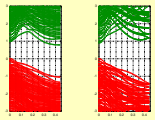
Silicon low-loss EELS

- 90°-partial glide dislocation, reconstructed SP structure
- No difference with bulk for low-loss EELS

Atomic structure



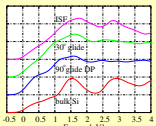




Dislocation Bulk

Silicon core EELS

- Internal stacking fault (ISF)
- 30°-partial glide dislocation
- 90°-partial glide dislocation, double period reconstruction (DP)
- Bulk



- Extra density for 90°-partial at 0.5 eV above CBM
- Small differences in peak positions

Conclusions

- EELS spectra can be qualitatively predicted by our level of theory
- Shuffle dislocations in diamond—rather than fully-reconstructed glide dislocations—show strong changes in EELS spectra
- Low-loss EELS:
  - not sensitive to reconstructed dislocations
  - most useful if there are empty levels in the gap
- Core-excitation EELS:
  - more sensitive to local bonding due to strong localization of initial state

References

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