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Improving detector-grade SiC by defect engineering: a first principles study

T.A. Oliveira, J. Coutinho, V.J.B. Torres

Department of Physics & i3N, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal

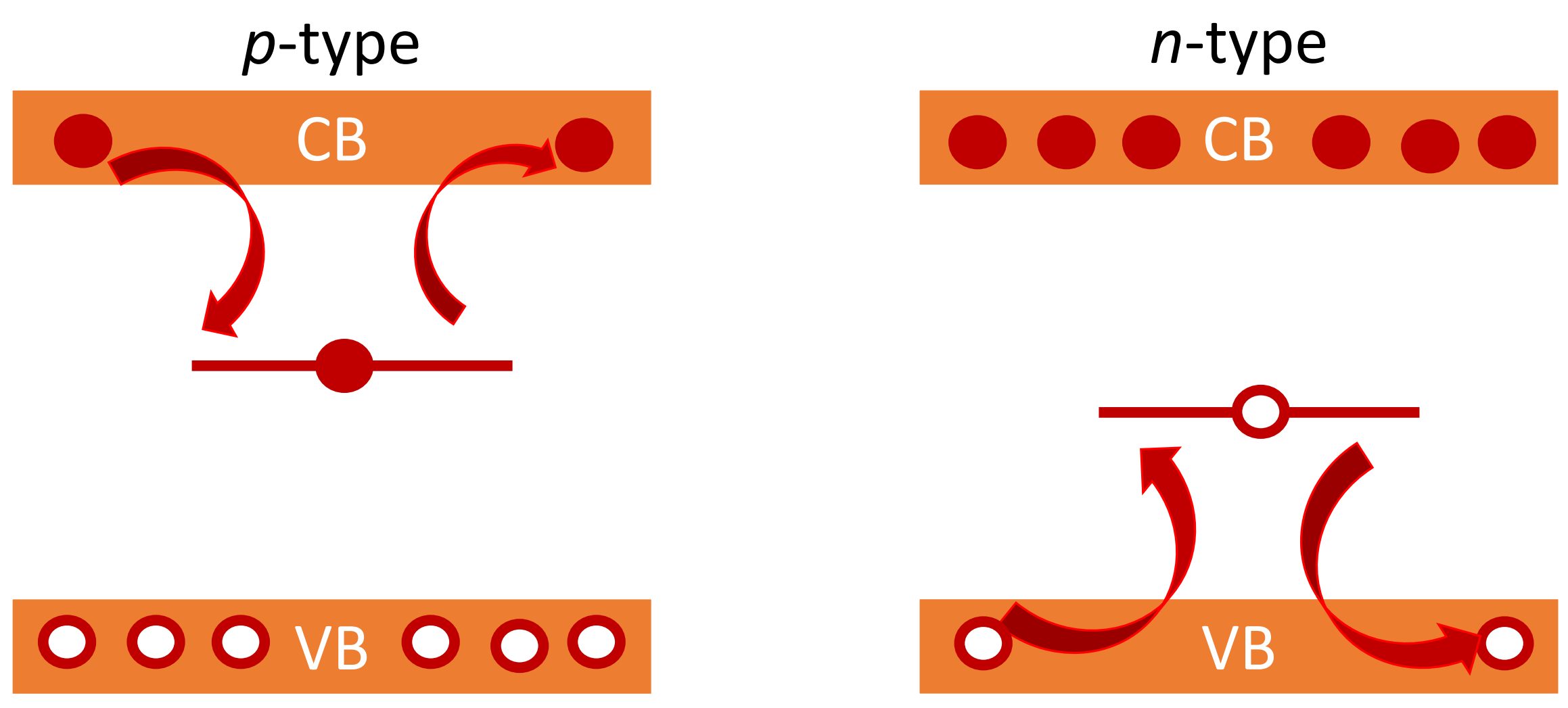
Silicon carbide (SiC), one of the most promising wide-bandgap (2.0 eV ≤ E_g ≤ 3.4 eV) semiconductors for making devices to be subject to harsh (high-temperature, highly corrosive, and high-radiation) environments [1]. It is also known that grown-in carbon vacancies have a huge impact in limiting the minority carrier life-time of SiC, and therefore they are highly detrimental to the performance of SiC as a base-material for radiation and light detection. Based on recent indications that SiC-growth based on a chlorinated chemistry strongly decreases the presence of carbon vacancies [2], we started to investigate by means of atomistic first-principles methods, what are the most stable complexes involving isolated Cl, F, H and O defects in 4H-SiC (the polytype of choice for making detector diodes), as well as their interactions with intrinsic defects like the carbon and silicon vacancies. We show that oxygen is a promising passivation agent of carbon vacancies, particularly in *n*-type material, where it either behaves as a double donor or as an inert interstitial impurity. We also found that interstitial oxygen impurities can be introduced in the SiC and be made to react with the vacancies at moderate annealing conditions.

Goal

- Increase efficiency in SiC-based radiation detectors.

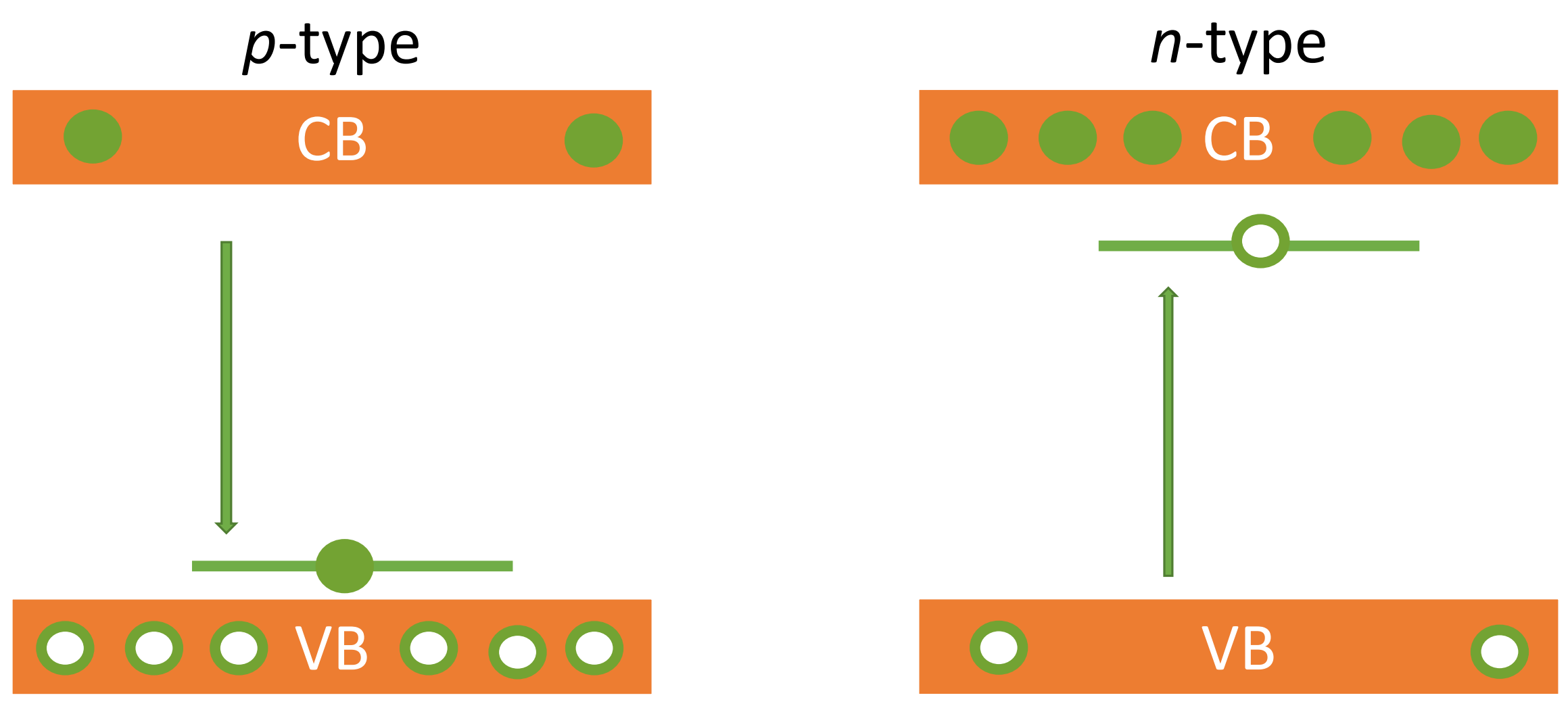
Major drawback

- Low minority carrier lifetime due to *deep*-level defects (e.g. carbon vacancy).



Proposed solution

- Improve minority carrier lifetime, introducing *shallow*-level defects.



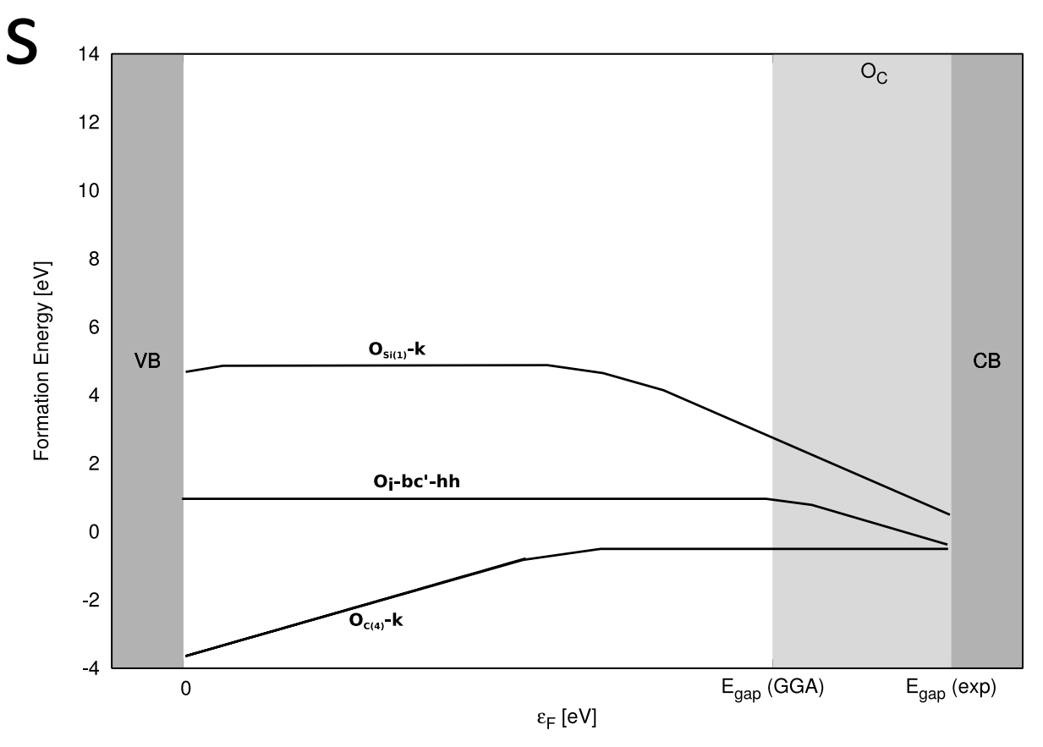
Method

- Density functional theory (DFT)[5-6] calculations with VASP code[9-12].
- *Ab initio* calculations with 576-atom supercells.

Oxygen in 4H-SiC

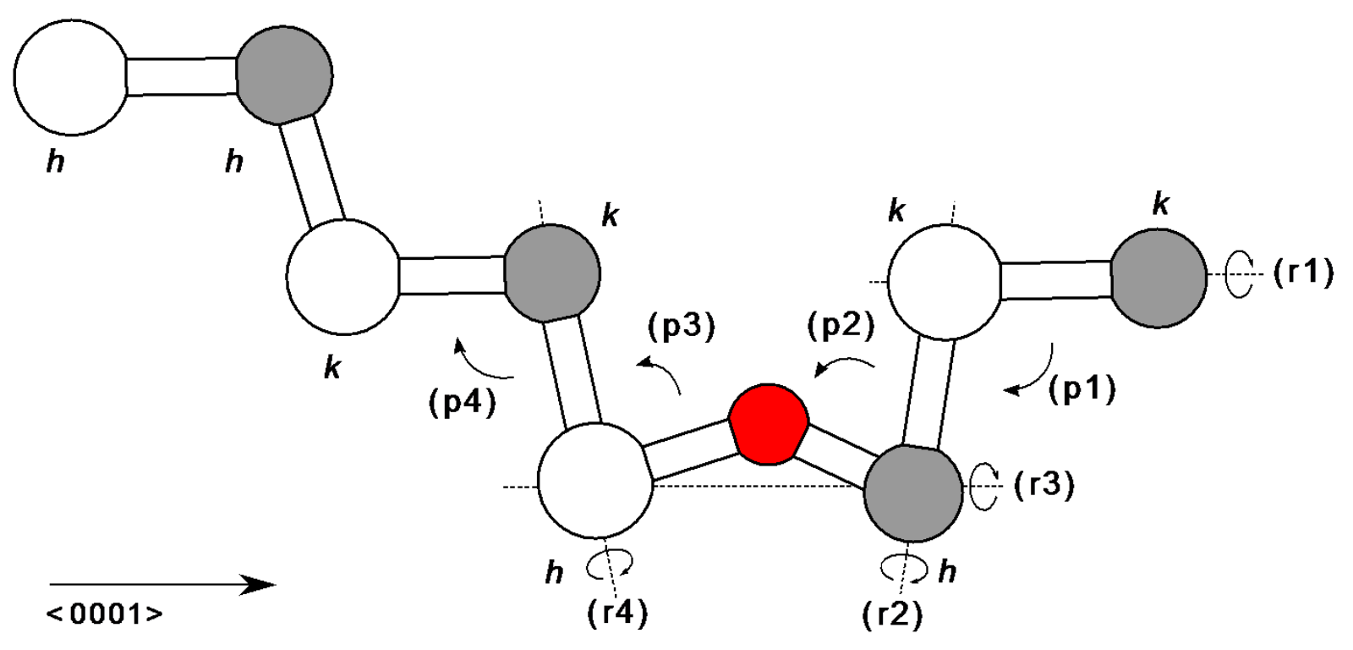
Defect formation energies:

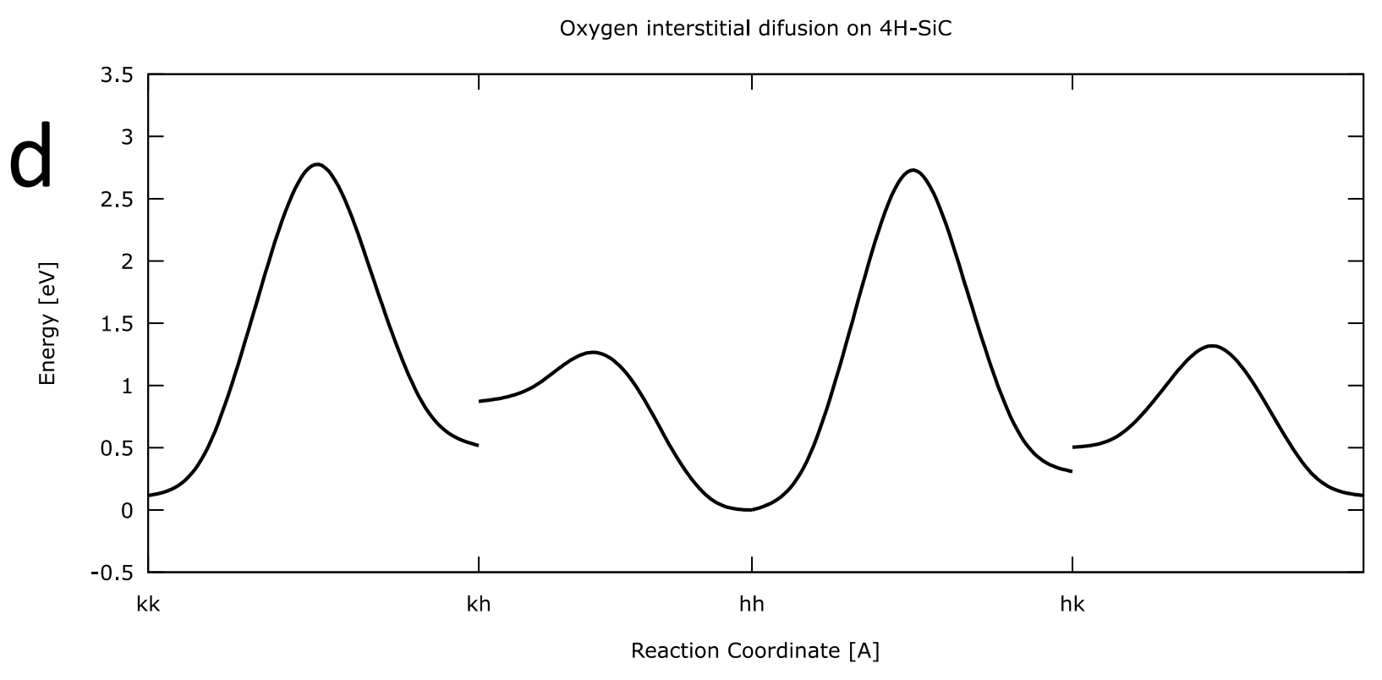
- Great variety of oxygen-related defects can exist at room temperature (substitutional and interstitials).
- Some defects present both donor and acceptor levels within the gap (e.g. $O_{Si(1)}$-k).
- O_i-bc'-hh (oxygen interstitial) present a *shallow* donor state that needs to be access using more accurate, and more computer costly, hybrid functionals.



Defect migration:

- The migration mechanism for the oxygen interstitial is depicted on the right.
- From the nudged-elastic method (NEB) we show that the major energy barrier (2,7 eV) needed for defect migration is due to O-C bond breaking.





Conclusions

- Oxygen is a common contaminant during SiC production.
- Oxygen-related defects show relatively low formation energy and huge variety of defect levels within the energy gap.
- Oxygen-related defects also have low migration barrier, witch can be easily overcome by annealing.
- Controlling which oxygen defects are formed during SiC grow and therefore witch defect levels will be present in the energy gap can result in improving the minority carrier lifetime.
- Ultimately, we show that oxygen defects can be an effective carbon vacancy passivation agent in SiC.

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