How semiconductor lasers fail – understanding recombination-enhanced dislocation climb mechanisms

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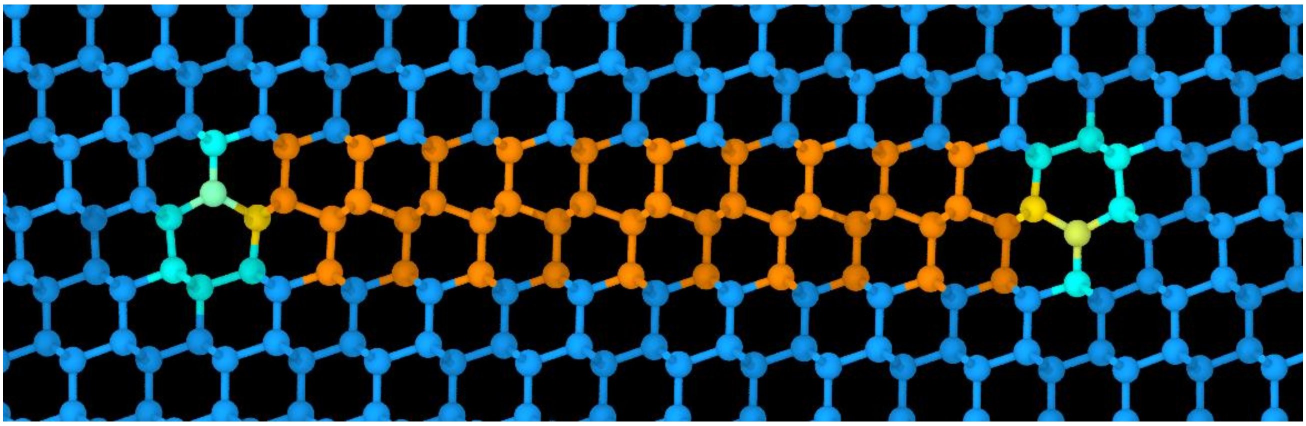
If a dislocation is present in the active volume of a light emitting device, it causes failure by acting as a carrier recombination pathway and grows through the material by emitting atoms, eventually quenching all luminescence. Despite the significant technological progress improved knowledge would generate, the atomistic mechanisms underlying this recombination-enhanced mechanism of dislocation climb and its interaction with vacancies and interstitials are poorly understood, with no first principles work reported to date. This PhD project will address this deficiency for the first time.



We will study two common dislocations found in semiconductors and FCC metals, both of which dissociate into two Shockley partial dislocations linked by an intrinsic stacking fault: (i) the 1/2<111> screw dislocation, which dissociates into two 30 degree partials (ii) the 60 degree dislocation, which dissociates into a $30°$ and a $90°$ partial. Experimental observations of climb of $60°$ dislocations in semiconductors invariably show that the $90°$ partial climbs by adsorbing interstitials, with no climb of the $30°$ partial; however, no atomistic mechanism has not been identified.

Dislocation climb is extremely challenging to address with conventional first principles approaches due to the simultaneous need for highly accurate models and large model systems, which have largely restricted theoretical work to individual dislocation cores [1]. This project will overcome this limitation using new theoretical tools that allow dislocation cores to be modelled with quantum mechanical precision and in a much larger atomistic medium [2]. A first step will be to predict the stacking fault length in case (i) and compare with experiment, before moving to the more challenging case of interstitial-driven climb in system (ii).

The success of the project will rely on close interaction between atomistic simulations and the atomic-resolution TEM capabilities in Richard Beanland's group. Data is already available for dislocation systems in III-V optical devices and diamond. During the PhD project more data will be collected in FCC metals (e.g. Al, Ni) to explore whether a universal mechanistic model for dislocation climb can be proposed and validated.

[1] D. Rodney, L. Ventelon, E. Clouet, L. Pizzagalli, and F. Willaime, Acta Mater. **124**, 633 (2017).
[2] P. Grigorev, T. D. Swinburne, and J. R. Kermode, Phys. Rev. Materials **4**, 023601 (2020).