Alexander Thorsten Blumenau, *The Modelling of Dislocations in Semiconductor Crystals*.
PhD Thesis (English), Department of Physics, Faculty of Science, University of Paderborn, Germany (2002).
140 pages, 70 figures, 14 tables.

Abstract

This thesis studies dislocations in semiconductor crystals by means of theoretical modelling. In particular, the work presented is focussed on dislocations in diamond and silicon carbide and addresses technologically relevant effects.

A thorough description of dislocation effects covers a wide range of length scales and requires a rather precise modelling of the electronic structure of a small core region at one end to long range elastic effects at the other end of the scale. This can hardly be achieved with one method only. Therefore, it is one of the main objectives of this work, *to give a more complete description of dislocations in semiconductor crystals by combining different theoretical methods*: Density functional theory (DFT) forms the basis for quantum mechanical atomistic calculations. Within DFT a pseudopotential approach is used to obtain electronic structures. A more approximate and far less computationally expensive DFT-based tight-binding method allows the prediction of core structures and energies embedded in larger models, representing a more extended region of the crystal. And finally, linear elasticity theory enables one to describe long range elastic effects at almost no computational costs.

After introducing the methods to be used and presenting the basics of dislocation theory, the dislocations of the $\{111\}\langle 110\rangle$ slip system in diamond serve as an example of how the different methods are combined in this work. Straight perfect as well as dissociated dislocations are investigated. The resulting low energy core geometries can be used as input coordinates for the simulation of high-resolution transmission electron microscopy images, and the calculation of the electronic structure allows the modelling of electron energy-loss spectra. Both are compared with experimental data.

Furthermore, the thermally activated glide motion of Shockley partial dislocations in diamond is modelled in a process of kink formation and migration.

Summarising, the results obtained support an annealing scenario for natural brown diamond involving a transition from shuffle to glide character at the dislocation core, which might explain the decolouring observed under high-pressure, high-temperature treatment — a process still not understood, but of utmost interest to the international diamond trade.

In modern silicon carbide technology a mechanism of recombination-enhanced dislocation glide is believed to play the key role in the observed disastrous degradation of bipolar devices under forward bias. To shed some light on this mechanism, in this work the different partial dislocations involved and their glide motion are modelled. The resulting electronic structures and glide activation energies are then directly related to recent experimental observations.

Keywords

dislocations, diamond, silicon carbide, SiC, density functional theory, elasticity theory

PACS

`61.72.Lk` Linear defects: dislocations, disclinations
`61.72.Bb` Theories and models of crystal defects
`61.72.-y` Defects and impurities in crystals; microstructure
`71.15.Nc` Total energy and cohesive energy calculations
`71.55.-i` Impurity and defect levels
`61.72.Ff` Direct observation of dislocations and other defects