Quantum mechanical analysis of changing surface elements on Silicon Carbide at extreme temperatures

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Introduction

Silicon Carbide is an exciting material with features that make it favourable to other conventional elements like Silicon in the power electronics field. It is an expensive material found rarely in nature, so being able to use computer models to simulate its structure and properties saves on cost and laboratory time.

It is not however, without its issues. A Silicon atom is slightly electronegative meaning it attracts electrons, and a Carbon atom is slightly electropositive meaning it repels electrons. This creates small electric fields across each Silicon and Carbon pairing, giving the effect of a much larger electric field across the entire structure (dipole effect). This electric field makes it difficult to calculate important properties of Silicon Carbide like its work function and electron affinity when modelled in this fashion.

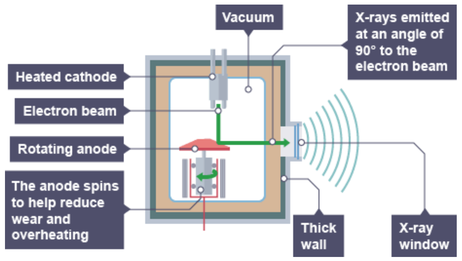

Figure 1 – Process of thermionic emission, generating electron beam

A materials Work Function tells us how much energy is required to remove an electron from its surface to a distance outside the surface, and Electron Affinity is how much energy the structure gains or loses when it absorbs an electron from outside the surface.

If we could overcome Silicon Carbide's dipole effect, and the electron emission properties were concluded to be superior, then its use in areas such as displays, thermo-tunnelling, and x-ray generation could increase.

Figure 2 – "Blob" of Silicon Carbide

Aims

- Simulate Silicon Carbide using AIMPRO software and add terminations to a non-polar surface
- Allow the software to optimise the positions and calculate the electrostatic potential through the structure and into the vacuum
- Plot the results and use these to calculate the emission properties
- Evaluate the viability of this method

Method

The aim was to create data files using AIMPRO that sets out how the Silicon Carbide is structured in real-space and the different parameters that control the structure's electrical properties. In an attempt to overcome the electric field, non-polar surfaces in a different direction were considered. In this direction, the electric field has no effect.

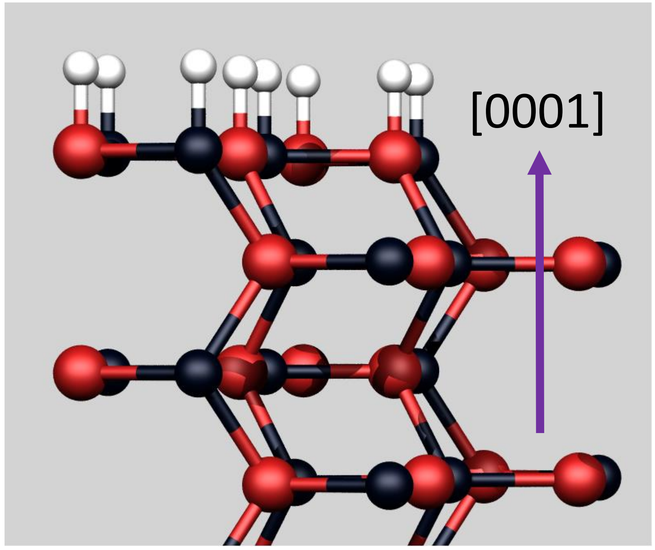

Figure 3 – Hydrogen terminated Silicon Carbide (Hydrogen: White, Silicon: Red, Carbon: Black)

A layer of halogen elements were also added to the surface of the material such as Hydrogen, Oxygen, Bromine, and Chlorine which are known for making a material's emission properties more favourable. The position of the atoms were optimised so that the forces they exert on each other are minimised along with the total energy of the structure. Once the positions have been optimised the electrostatic potential through the material was calculated.

Results

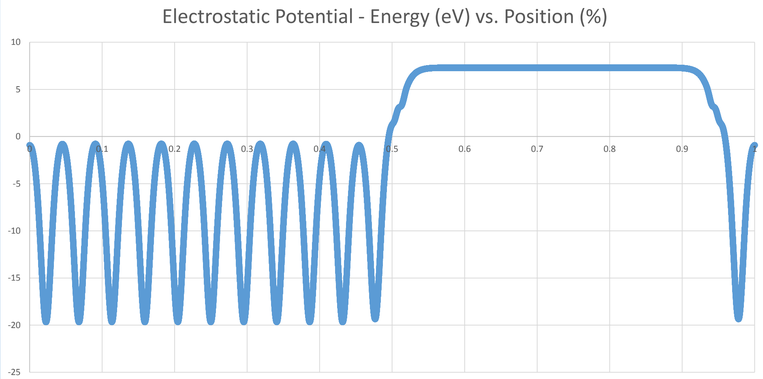

Figure 4 – Result of the simulation calculating the electrostatic potential

The graph shows how the energy changes from the top layer of the structure through to the bottom and then out in to the space between structures. The sinusoidal part (wavy section) shows how the energy changes periodically through the structure because of its symmetry. The energy then increases and levels off, representing an important property called the vacuum potential. This is the energy of the near surface space outside the structure, and is a crucial reference point when calculating the field emission properties.

Hydrogen and Hydroxyl terminations have lower work functions with values of 9.21eV and 9.94eV respectively, and also lower electron affinities with values of 1.59eV and 2.84eV respectively. Harsher terminations such as Chlorine and Fluorine had overall higher results, with work function values of 10.45eV and 12.32eV respectively, and electron affinities with values of 3.85eV and 3.97eV respectively.

This non-polar surface has proven to be viable for field emission, allowing people to decide whether or not this is a material whose properties suit the application of the product they are designing.

Conclusions

- This method produces a well defined vacuum potential, completely avoiding the effect of the electric field
- Silicon Carbide has been found to have a relatively high work function and electron affinity
- The success of the variation opens up the potential for future research into other field cancelling methods

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References: Figure 1 – http://www.bbc.co.uk/schools/gcsebitesize/science/triple_edexcel/xrays_ecgs/xrays/revision/3/

Figure 2 - David.Monniaux - https://en.wikipedia.org/wiki/Silicon_carbide#/media/File:SiC_p1390066.jpg