NON-LINEAR AND PIEZO ELECTRONIC PROPERTIES OF GALLIUM NITRIDE

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ABSTRACT

With the advent of the laser in 1960 a resurgence in the study of non-linear response in materials occurred, which has been ongoing to this very day. Modern technology heavily utilises non-linear properties of materials, from the DC-Pockels effect which is used to modulate devices, such as LCD displays and pulsed lasers, to the many different type of frequency mixing, such as second order harmonic generation (SHG) which for one can be used to generate light of otherwise hard to achieve frequencies [1].
These effects rely on the susceptibility of materials, and as new materials join the roster of electronics in the continued development of the modern world it is crucial to map the properties these materials. One such material is gallium nitride (GaN) which is of particular interest in power electronics owing to its high operational temperature and switching speed, among other reasons [2].
GaN also feature a large, direct bandgap making the material ideal for optical devices as well. However, due the lattice mismatch of substrates, defect states and stress are introduced which alters the properties of the material and must therefore be accounted for [3].

In this paper, ab initio methods in the form of density functional theory, implemented using GPAW, will be utilised to determine the first and second order susceptibility of GaN. The calculations will be augmented by the scissors method to achieve the correct band gap, and the tetrahedral method to reduce computational time. If possible, SHG experiments on a 0.5 mm m-plane GaN sample at temperatures between 170 and 290 Kelvin will be conducted. Additionally, the piezoelectric tensor will be calculated and experimentally tested.

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