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Electronic defects in $LaAlO_3$

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Abstract

We present calculations of the energy levels of the oxygen vacancy, the Al_{La} antisite and the oxygen interstitial defects in $LaAlO_3$ using density functional methods that do not need an empirical bandgap correction. The levels are aligned to those of the Si channel using the known band offsets. The oxygen vacancy gives an energy level near the $LaAlO_3$ conduction band and above the Si gap. It is identified as the main electron trap and a cause of instability. There is only one vacancy level in the gap, because the higher second level lies within the La conduction band. The Al_{La} antisite gives a state near midgap, neutral when empty, which would be an important trap, with no counterpart in HfO_2.
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1. Introduction

The continued scaling of complementary metal oxide semiconductor (CMOS) transistors requires the replacement of the SiO_2 gate oxide by dielectrics of a higher dielectric constant (κ) to minimise leakage currents [1,2]. Presently, the leading high K oxide is HfO_2 and its alloys. However, HfO_2 layers on Si tend to possess a SiO_2-based interfacial layer which limits the attainment of very low effective oxide thickness (EOT). Future scaling calls for lower EOTs, and for this a leading candidate is $LaAlO_3$ [3–15].

$LaAlO_3$ is thermally stable in contact with Si. But a key advantage of $LaAlO_3$ is that it has much lower atomic diffusion rates than HfO_2, which limits the growth of any subcutaneous SiO_2 layer between the Si channel and the oxide [12–14]. Recently amorphous $LaAlO_3$ gate stacks with an EOT of only 0.3 nm were achieved [15].

A second factor is that amorphous gate oxides are still preferred, because they are isotropic and do not contain grain boundaries which act as short circuit diffusion paths. The lower diffusion rates of $LaAlO_3$ lead to a higher crystallisation temperature, and indeed $LaAlO_3$ does not crystallise until 850 °C [7], even without the addition of nitrogen. However, amorphous $LaAlO_3$ appears to have a lower K value than the crystal [4].

A third factor is that La-based oxides have higher conduction band offsets than Hf oxides, because of La's lower valence [16–21]. This reduces leakage currents and extends the scaling performance of $LaAlO_3$.

Crystalline $LaAlO_3$ has the perovskite structure, like $SrTiO_3$. Much of the work on $LaAlO_3$ on Si has been motivated by desire to grow epitaxial $LaAlO_3$ on Si [11,12,22–24]. This is based on the close lattice match of cubic $LaAlO_3$ to Si, with the (100)$LaAlO_3$||(100)Si and [110]$LaAlO_3$||[100]Si. However, presently, $LaAlO_3$ films grown on Si are amorphous, unless a few layers of $SrTiO_3$ on top of the Si are used as a template layer. On the other hand, Si can be grown on $LaAlO_3$ [22].

$LaAlO_3$ differs from $SrTiO_3$ in that it is a 3–3 valent perovskite rather than a 2–4 perovskite. As La and Al have the same valence, this means that La and Al antisites are possible defects, and the ability of La and Al to mix sites could be a cause of the films growing as an amorphous phase.

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The introduction of high *K* oxides in CMOS has been delayed partly because of their high defect concentrations, particularly O vacancies. These vacancies result in charge trapping, transient threshold voltage shifts, and a contribution to lower Si carrier mobility due to remote Coulombic scattering. It is therefore important to have a good prediction of defect properties, particularly defect energy levels, as these determine the amount of any charge trapping.

2. Calculation method

This paper presents calculations of the defect levels of $LaAlO_3$ following our initial work, and discusses the reasons for the difference to HfO_2. There have previously been a number of calculations of the bulk, interfaces and defect energy levels of HfO_2, using the local density approximation (LDA) or its later development, the generalised gradient approximation (GGA) [17,25–29]. LDA and GGA give good values of the ground state properties such as lattice constants and elastic moduli. However LDA and GGA are well known to underestimate the bandgap of insulators. In some cases, this can be a sizable effect. It is possible to correct this empirically for the bulk material, by a simple rigid upward shift of the conduction bands. But this is less reliable for gap states. It is preferable to use methods beyond the simple LDA which give correct bandgaps [26]. These methods include the GW approximation, B3LYP, LDA plus U, screened exchange (sX), and weighted density approximation (WDA). In this paper, we use the sX and WDA methods [30], as recently summarised [26].

The calculations model the defect using a supercell of 40–80 atoms of cubic $LaAlO_3$, containing a single vacancy, interstitial or antisite. The defect structures are relaxed in their various charge states using the PBE version of GGA using ultra-soft pseudopotentials. The defect energy levels are then calculated with the sX method, using norm-conserving pseudopotentials with a cut-off energy of 600 eV. The antisite and interstitial levels are also calculated in WDA with ultra-soft pseudopotentials and a cut-off energy of 400 eV. sX is more accurate than WDA, but WDA allows us to use larger supercells, which are needed when there are large atomic relaxations around the defect.

3. Results

$LaAlO_3$ has the ABO_3 perovskite lattice, with a lattice constant of 3.78 Å. The oxygens are surrounded by two Al atoms. Unusually, the transition metal/rare earth La ion is at the A site, surrounded by 12 oxygens, and the main group ion Al is at the B site surrounded by six oxygens. In the amorphous phase, Al is part of the covalent network – a network former – while La is an interstitial ion – a network modifier. The fact that Al and La have the same valence means that the antisite defects might be possible. The equivalent question in the amorphous phase is how much Al or La find it energetically preferable to be network former or modifier.

Fig. 1 shows the band structure and Fig. 2 shows the partial density of states (DOS) of bulk cubic $LaAlO_3$. The bandgap is indirect, from R in the valence band to Γ in the conduction band. The valence band is formed mainly of O 2p states, and the lowest conduction band is due to La d states with the Al s, p states forming a higher conduction band above 9 eV. This is a key result for later; the lowest conduction band is on the La ions (A ions), not the Al ions (B ions), in contrast to many other perovskites. The bandgap of bulk $LaAlO_3$ is calculated to be 3.1 eV in GGA, 4.4 eV in sX and 6.7 eV in WDA, compared to 5.6 eV experimentally [18,19]. Unlike in HfO_2 where the sX, WDA and experimental gaps are similar, the sX gap of $LaAlO_3$ is smaller than the WDA or experimental gap.

Turning to the defects, consider first the oxygen interstitial, denoted I. I^{2-}, the O^{2-} interstitial ion, is a closed shell system. It is well separated spatially from other O^{2-} ions.

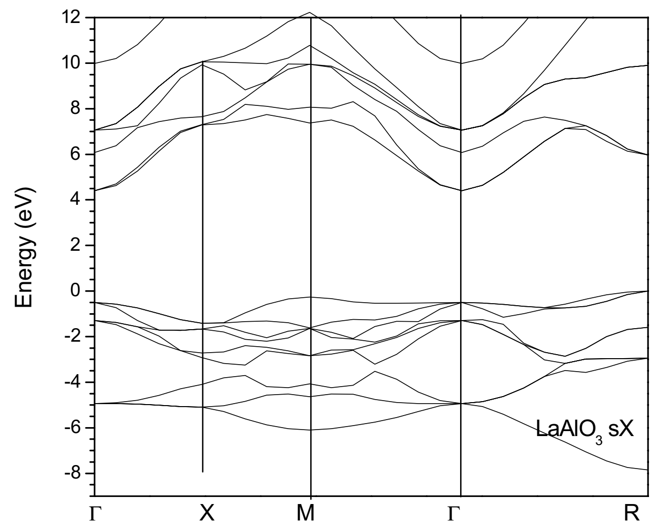

Fig. 1. Band structure of cubic $LaAlO_3$ by screened exchange.

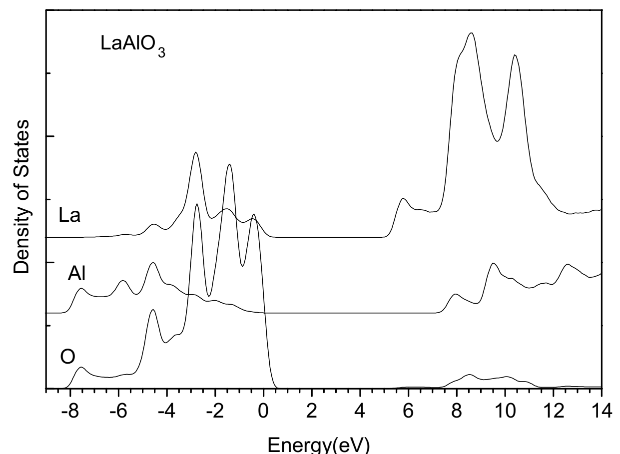

Fig. 2. Partial density of states of $LaAlO_3$.

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