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Oxygen vacancy migration in compressively strained SrTiO₃

Raied Al-Hamadany,^{1,a)} J. P. Goss,¹ P. R. Briddon,¹ Shahin A. Mojarad,¹ Meaad Al-Hadidi,¹ A. G. O'Neill,¹ and M. J. Rayson²

¹*School of Electrical and Electronic Engineering, Newcastle University, Newcastle upon Tyne NE1 7RU, United Kingdom*

²*Department of Engineering Sciences and Mathematics, Luleå University of Technology, Luleå S-97187, Sweden*

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The intrinsic properties of strontium titanate render it promising in applications such as gate dielectrics and capacitors. However, there is growing evidence that oxygen vacancies significantly impact upon its use, with the diffusion and deep donor level of the oxygen vacancy leading to electrical leakage. Where grown epitaxially on a lattice mismatched substrate, SrTiO₃ undergoes bi-axial strain, altering its crystal structure and electronic properties. In this paper, we present the results of first-principles simulations to evaluate the impact of strain in a (001) plane upon the migration of oxygen vacancies. We show that in the range of strains consistent with common substrate materials, diffusion energies in different directions are significantly affected, and for high values of strain may be altered by as much as a factor of two. The resulting diffusion anisotropy is expected to impact upon the rate at which oxygen vacancies are injected into the films under bias, a critical factor in the leakage and resistive switching seen in this material. © 2013 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4775397>]

I. INTRODUCTION

Metal-oxides are used extensively in electronics, exploiting a number of physical properties that are required for different technological applications. For example, in the ongoing improvement in functionality of silicon-based integrated circuits, the native dielectric (SiO₂) must be replaced with high- κ materials. Several high- κ binary (e.g., HfO₂, TiO₂, and Al₂O₃) and ternary (e.g., SrTiO₃ and BaTiO₃) metal oxides have been proposed for this role.¹ Since the critical factor is their high permittivities, crystalline SrTiO₃ is well placed with ϵ_r being² around 300 at room temperature. Indeed, SrTiO₃ has been demonstrated in capacitive,³ resistive switching,^{4–7} and gate applications.⁸

A large body of work, both the experimental and theoretical, has been directed toward an explanation for the origin of leakage current and the mechanisms underlying resistive switching.^{7,9–12} The majority of models feature oxygen vacancies, V_O , in a central role.^{7,12–15}

Importantly, although the involvement of V_O in the electrical and other properties of SrTiO₃ films inferred from experiment may be largely circumstantial, the electronic, electrical, thermodynamic, and kinetic properties of V_O have been established using quantum-chemical simulations.^{16–20} Under oxygen lean conditions, V_O has a lower formation energy compared with other native defects.¹⁷ The electrical conductivity ascribed to V_O is associated with the double-donor activity of the center,^{20–22} although the precise location in the band gap remains uncertain. Experimental estimates suggest that V_O is relatively shallow donor²³ with a level 0.24 eV below the conduction band edge. Calculated values vary significantly, with simulation method and system size probably

being the root cause of the variation. For example, density functional calculations yield single and double donor levels around 0.77 and 1.20 eV below the conduction band,²⁴ whereas recent supercell simulations²⁵ using large supercells yielding values of 0.40–0.50 eV.

In addition to the electrical levels, theory has also yielded quantitative estimates relating to the diffusion of V_O . The oxygen ions in cubic SrTiO₃ are sited octahedrally around titanium ions. The generally accepted migration mechanism for V_O involves the vacancy moving between sites adjacent to a common Ti. Since oxygen ions in SrTiO₃ are equivalent by symmetry, V_O migration mechanism is symmetrical between any two oxygen sites. It has been found that V_O diffuses relatively easily in comparison with other native vacancies in bulk SrTiO₃.^{18,19} Anelastic relaxation experiments suggest a barrier of 0.98 eV,²⁶ while recent isotope diffusion yields a lower value of 0.60 eV.²⁷ Both estimates are lower than the experimental values of 2.80–4.00 eV and 3.30–4.90 eV for Sr and Ti vacancies, respectively.^{28–30} Computational estimates^{17–19,25,31} for the barrier to diffusion of V_O range between 0.40 and 0.9 eV.

In addition to compositional effects, strain caused by epitaxy on substrates with different lattice constants is another source of significant modification of the electronic properties of perovskites.³² Among common substrate materials, bi-axial compressive strains for SrTiO₃ of around 1.8% (Rh³³ and KTaO₃³⁴), 3% (LaAlO₃),³⁵ and 7% (ZrO₂:Y₂O₃)³⁶ might be expected. Bi-axial strains alter the crystal and electronic structures of SrTiO₃ differently depending upon the direction and magnitude of strain,^{37,38} and, in principle, the dielectric constant can be optimized by control of the strain.³⁹ A key to the differences observed in bi-axially strained SrTiO₃ with different signs of strain is the different ferroelectric phases generated.⁴⁰ Compressively strained SrTiO₃ with strain range

^{a)}r.a.s.al-hamadany@ncl.ac.uk.

(3%–9%) has been previously simulated⁴¹ to investigate the effect of strain upon the rotation of oxygen polyhedral around the [001]-axis. According to the study, there was an increase in the rotation angle for strain values up to 5%, but absent at high strain. The internal structure changes with strain are qualitatively the same as ferroelectric phase transitions, and the displacements of one sub-lattice relative to another, in general, lower the symmetry, leading to non-equivalent oxygen sites in the lattice, and hence non-equivalent V_O centers.

For a clear picture of oxygen vacancy transport in thin film SrTiO_3 , it is, therefore, crucial to understand the mechanistic and quantitative impact of bi-axial strain upon the migration. Since extracting unambiguous data of this nature from experiment is extremely challenging, quantum mechanical modeling is an effective route to gain insight into the microscopic nature of oxygen vacancy migration in strained SrTiO_3 . In this study, we present results of atomistic, quantum-chemical modeling of SrTiO_3 under isotropic compressive bi-axial lattice strain in the (001) plane and the impact it has upon the oxygen vacancy diffusion.

II. COMPUTATIONAL METHOD AND MODELS

The calculations of oxygen vacancy migration in strained SrTiO_3 were executed using spin-polarized density functional theory (DFT) within the local density approximation,⁴² as implemented within the AIMPRO code.^{43,44} The use of this approach is supported by recent reports that show for SrTiO_3 ³⁷ and ZnO ⁴⁵ density functional simulations within the local-density approximation are suitable for prediction of trends as a function of strain.

Norm-conserving pseudopotentials were used to represent the core electrons,⁴⁶ where the valence sets are taken to be $4s^2 4p^6 5s^2$, $3s^2 3p^6 3d^2 4s^2$, and $2s^2 2p^4$, for Sr, Ti, and O, respectively. Kohn-Sham eigen-states are expanded using atom-centered Gaussian basis functions⁴⁷ as follows: Sr is treated using five independent sets of *s*- and *p*-Gaussians, yielding 20 functions per atom. Titanium and oxygen are represented using four sets of *s*-, *p*-, and *d*-Gaussians yielding 40 functions per atom. Matrix elements of the Hamiltonian are determined using a plane wave expansion of the density and Kohn-Sham potential⁴⁸ with a cutoff of 300 Ry, which yields well converged total energies with respect to this parameter. The same basic approach has been successfully used to investigate⁴⁹ the impact of water adsorption on SrTiO_3 .

We model SrTiO_3 epitaxially grown onto cubic substrates with lattice constants less than that of SrTiO_3 , where the substrate is included in the calculation only through the lattice matching. We have also assumed an isotropic in-plane strain so that the resulting unit cell geometry of the SrTiO_3 is tetragonal. The unit cell of SrTiO_3 then possesses an in-plane lattice constant of *a* equal to that of the substrate, and the perpendicular lattice constant, *c*, is chosen to minimise the total energy under the in-plane constraint. Although strains up to around 4% are typically considered in strained SrTiO_3 and related materials in calculations,^{37,40} in order to cover the wide range of lattice mismatch between SrTiO_3 and typical substrate materials yielding a compressive strain, five values of *a* have been simulated: in addition to unstrained material, values of

compressive strain of 2%, 4%, 6%, and 8% have been included in this study, and we note that strains in excess of this range have previously been included in computational studies.⁴¹

The (001) biaxial-strain breaks the symmetry of cubic SrTiO_3 , rendering sets of oxygen sites inequivalent. It then becomes convenient to distinguish oxygen atoms as lying in a (001) plane where the metal ions are entirely Ti or Sr, as shown schematically in Fig. 1(a). The lattice distortion also means that there are several distinct diffusion paths, all of which must be examined in order to fully characterize the diffusivity of V_O in strained SrTiO_3 .

V_O was simulated using large supercells with lattice vectors $[a\bar{a}c]$, $[\bar{a}ac]$, and $[\bar{a}\bar{a}c]$, where *a* and *c* are the lattice constants in the underlying tetragonal unit cell, so that in the unstrained limit *a* = *c*. This supercell is comprised from 32 formula units, so that in the case where V_O is present, the supercell is $\text{Sr}_{32}\text{Ti}_{32}\text{O}_{95}$. The strained bulk SrTiO_3 was modeled using a $2 \times 2 \times 2$ superlattice of primitive cells, $\text{Sr}_8\text{Ti}_8\text{O}_{24}$ with lattice vectors $2[a00]$, $2[0a0]$, and $2[00a]$. The use of a non-primitive cell is essential to allow for the possibility of antiferroelectric distortions, known to be present at very low temperature in pure SrTiO_3 , and induced under strain.

To establish an accurate and computationally tractable approach for our study, preliminarily calculations of V_O migration barrier in strain-free SrTiO_3 were carried out with two cell sizes (160 and 320 atoms) and different sampling densities. The calculated value from 320 atoms and Γ -point sampling was 0.61 eV which is in line with a previous calculation¹⁹ with the same system size and sampling at 0.53 eV. However, we find that the *Gamma*-point approximation is particularly poorly converged, even for the 320 atom cell: we have calculated the barrier to diffusion using a $2 \times 2 \times 2$ Monkhorst-Pack⁵⁰ mesh for the 320 atom cell size, and obtained 0.82 eV. We conclude that, although the activation energies we calculate are larger than this recent theory, the difference is likely to be a consequence of the sampling. In case of 160 atom cells, the Brillouin zone was either sampled using a $2 \times 2 \times 2$ mesh, or a single real *k*-point, located at the zone boundary, set half way along each reciprocal lattice vector. Under both schemes, the calculated migration barrier was calculated to be 0.81 eV, differing by less than 20 meV. Indeed, the zone-boundary point in the 320 atom cell also yielded 0.81 eV, confirming the quantitative accuracy of our approach. We conclude that the zone-boundary sampling is sufficiently converged, and we have used this throughout the calculations to render the simulations tractable. For the structural distortion of defect free SrTiO_3 , the 40 atom bulk cell was modeled using a $4 \times 4 \times 4$ sampling scheme, which represents a comparable density to that of the single point in the 160 atom cell.

Based upon the stated computational approach, the lattice constant of bulk (unstrained) SrTiO_3 is calculated to be 3.87 Å, which is in accord both with the experiment⁵¹ and previous calculations.⁴¹

For the calculation of the migration barrier, two methods have been employed; for the full minimum energy paths, we use climbing nudged elastic bands^{52,53} and under suitable

FIG. 1. (a) Schematic view of strained STO showing the sequence of SrO and TiO_2 (001)-planes parallel to the plane of strain. The oxygen sites 1–4 and 7–10 are within TiO_2 -planes, while sites 5 and 6 are within a SrO-plane. (b) Shows a projection onto the (001) plane of one unit cell under bi-axially compressive (001) strain, showing the four oxygen sites labeled 1–4 within a TiO_2 -plane. In both images red, gray, and yellow circles represent oxygen, titanium, and strontium ions, respectively.

circumstances we also estimated diffusion barriers using structural optimisation with a symmetry constraint. The use of symmetry was tested for selected systems by confirmation of the saddle point energy with the use of a full minimum energy path calculation. All the energy barriers in this study were optimised until forces on each image are less than 10^{-4} atomic units. A minimum of five images were used, with the convergence of the saddle point energy with respect to the number of images being established in each case.

III. RESULTS AND DISCUSSION

We first discuss the impact of strain upon the crystal structure of SrTiO_3 , and the consequences this have upon the migration routes proposed for V_{O} .

Consistent with recent calculations^{37,40} of strained SrTiO_3 , we find that under compressive bi-axial (001)-strain,

the oxygen sub-lattice is displaced along the [001] direction (normal to the plane of strain) relative to the cation sub-lattice, as shown schematically in Fig. 2(a). Thus, SrTiO_3 strained by isotropic compression in the (001) plane becomes ferroelectric distortion (FD) with a structure corresponding to the unstrained low temperature form of PbTiO_3 . In addition, there is an anti-ferroelectric distortion (AFD), consisting of a rotation of oxygen polyhedral about the [001]-axis as shown in Fig. 2(b). Such phase mixing under compressive strain has been previously reported,⁴¹ where the compressively strained SrTiO_3 displayed two energy minima under 5%–7% strain.

Table I details our calculated displacements, as specified in Fig. 2, and energies of FD and mixed FD + AFD phases relative to unstrained SrTiO_3 under each value of strain, E_1 , which is the cost per formula unit to produce the strained SrTiO_3 . In addition, the energy relative to a bi-axially strained

FIG. 2. (a) Schematic view showing the [001] displacement of the oxygen sub-lattice relative to the cation sub-lattice under compressive strain leading to ferroelectric distortion of SrTiO_3 along the [001] direction. (b) Shows the rotation of the TiO_6 polyhedral about the axis of compressive strain [001]. Colors of atoms are defined in Fig. 1.

TABLE I. Calculated parameters for isotropic bi-axial (001) strained SrTiO₃. Sub-lattice displacements D_{O-Ti} and D_{O-Sr} (Å) are defined in Fig. 2, the angle of rotation about the [001] axis is θ (degrees), and the c/a ratio is the equilibrium value obtained for the FD and FD + AFD structures constrained by the specified strain. Relative energies per formula unit (meV) are calculated relative to cubosymmetric, unstrained SrTiO₃ (E_1), and relative to biaxially strained SrTiO₃ constrained to a centro-symmetric structure (E_2) where the c/a ratio is not constrained to that of the distorted phase.

Strain (%)	D_{O-Ti}	D_{O-Sr}	Phase	θ	c/a	E_1	E_2
2	0.12	0.07	FD	...	1.03	55	-10
4	0.23	0.16	FD	...	1.05	232	-49
	0.17	0.10	FD + AFD	10.0	1.09	205	-75
6	0.41	0.19	FD	...	1.29	493	-185
	0.26	0.40	FD + AFD	13.7	1.20	448	-229
8	0.55	0.68	FD	...	1.35	734	-567

system constrained to a centro-symmetric symmetry, E_2 , is included to show a quantitative measure of the extent to which the internal structural re-organisation stabilizes the SrTiO₃. E_2 is negative as this is the energy gained by relaxation from a constrained, strained SrTiO₃ into the distorted phases. The large energies for high values of strain indicate that such material would be likely to be stable only in very thin films.

The AFD angles under compressive strain are large in comparison to the intrinsic, low-temperature⁵⁴ distortions around 2.1° in pure, unstrained SrTiO₃ (this relatively small angular effect has been reproduced in the current calculations for unstrained material, where we have obtained an angle of 1.98°). This low-temperature AFD is included in all zero-strain calculations. The impact of the AFD at zero strain upon the diffusion barriers and mechanisms, such as in the number of parts of a complete diffusion process, is extremely minor. This is in stark contrast with the strained material. For example, at 4% strain, the AFD angle is 10° and corresponds to a larger energy, so that first, it is expected to persist to much higher temperatures, and second the impact upon the mechanisms for diffusion is much more significant.

With reference to on Fig. 1(a), there are two planes for diffusion of V_O entirely within a (001) plane, identifiable as TiO₂ and SrO planes. The distance between oxygen sites within a TiO₂-plane (sites 1 and 2 in Fig. 1) is less than in a

SrO-plane (sites 5 and ion 6, Fig. 1(a)). Calculations have been performed for the corresponding paths in zero strain SrTiO₃, resulting in values of 0.81 eV and 4.18 eV for the TiO₂ and SrO planes, respectively. The migration barrier of V_O in the TiO₂ layer is in excellent agreement with the experiment⁵⁵ (0.86 eV) and with the previous calculations noting the variations due to cell size and sampling.^{19,31} In line with the observation that the neutral vacancy is less mobile than the ionized form,⁵⁶ we find that the barriers for the single and double positive charge state the migration barriers are 0.74 eV and 0.77 eV, respectively. The very high value of the activation energy for diffusion entirely within the SrO plane means that such mechanisms are unlikely to play a significant role in V_O diffusion, even in strained material. We, therefore, restrict the analysis in strained SrTiO₃ to mechanisms involving the diffusion of V_O between sites neighboring a common Ti ion site.

For diffusion between different (001) planes of atoms in the compressively strain SrTiO₃, there are two steps to complete full diffusion process. A characteristic path can be envisaged as V_O diffusing along the path 1–5–7, as labeled in Figs. 1(a) and 3. This can be viewed as the vacancy moving from planes of TiO₂ to SrO and returning to TiO₂, for which we adopt the notation Δ_{1-5} and Δ_{5-7} .

We now present the results of the analysis for the diffusion processes first within the (001)-plane, and then inter-(001)-planes.

A. In-plane migration of V_O

The in-plane migration barrier for the three charge states of V_O as a function of compressive strain is plotted in Fig. 4. We find that up to around 4% strain, the migration energy varies only very slightly, but above this strain value there is clear drop in the barrier. We note that the behavior is very similar for all three charge states. The general reduction in activation energy can be understood as the distance between the oxygen sites becomes closer with increasing strain.

The small variation of the energy barrier up to 4% reflects the similarity of the diffusion mechanism under these values of strain (2% and 4%) and the diffusion in zero strain cubic SrTiO₃. At high values of strain (6% and 8%), the

FIG. 3. Schematic illustration of (a) equivalent in-plane diffusion paths (Δ_{1-2} , Δ_{2-3} , Δ_{3-4} , and Δ_{4-1}) and (b) two non-equivalent, inter-plane diffusion paths, Δ_{1-5} and Δ_{5-7} . The isotropic bi-axial strain is within the (001) plane.

FIG. 4. The in-plane V_O migration barrier as a function of isotropic, (001)-plane bi-axial compressive strained, corresponding to the path Δ_{1-2} in Fig. 3(a). Circles, triangles, and squares refer to neutral, +1, and +2 charge states, respectively.

displacement of the oxygen ions from the titanium layer becomes a significant factor, resulting in a reduction in the energy barrier.

B. Inter-plane migration of V_O

For the inter-plane diffusion, a full migration trajectory requires (at least) two steps in the distorted phases, labeled Δ_{1-5} and Δ_{5-7} in Fig. 3. The non-equivalence of V_O in the TiO_2 and SrO planes is reflected in an energy difference in favor of the TiO_2 plane by 61 meV, 77 meV, and 93 meV in the neutral, +1, and +2 charge states, respectively, at 2% strain.

Under high strains (above 4%), the structure of V_O in the SrO plane cannot be described as a single missing oxygen ion. Instead, there is a relaxation over the neighbouring sites in the adjacent TiO_2 plane, as shown schematically in Fig. 5(b). Here, the vacancy can be viewed as lying at site 5 in Fig. 5(b), and the oxygen ions at site 7 and 9 move significantly, approximately in the $[00\bar{1}]$ direction. A similar distortion has been proposed previously for unstrained LaMnO_3 .⁵⁷

The existence of the structural distortion above 4% leads to the possibility for a reorientation process involving the pair of O-sites that relax toward the vacancy in the SrO -plane. The two possible arrangements involve the $[00\bar{1}]$ displacements of either sites 7 and 9, or 8 and 10 in Fig. 1(a). Reorientation between these configurations does not represent a necessary stage in the inter-plane migration, but could conceivably be a stage in a process where V_O alternates between the same TiO_2 and SrO planes. We find, however, that the barrier for reorientation is not the rate limiting step for inter-plane diffusion, with calculated activation energies of 1.0 and 0.7 eV at 6% and 8% compressive strain, respectively.

1. The Δ_{1-5} step

Figs. 6(a), 6(c), and 6(e) plot the migration barrier as a function of compressive strain for the first stage of inter-plane diffusion, labeled Δ_{1-5} in Fig. 3(b). The diffusion barrier varies in two phases with increasing strain: initially, (up to 4%) the activation energy increases for all charge states, but for higher strains the barrier diminishes, so much so that by 8% the activation energy is less than that in unstrained material.

This behavior may be explained based upon two factors. First, the bi-axial compressive strain within the (001)-plane yields an elongation in the inter-ion distances in the $[001]$ direction. Such elongation leads to greater spacing between the atomic planes along $[001]$ direction. The increased distance that the V_O has to traverse between planes tends to increase the activation energy, and for strains up to 4% this is the dominant factor.

Second, the existence of structural rearrangements in the SrO plane (see Fig. 7) reduces the cost of the final point in the Δ_{1-5} path, so that above 4% the distance and energy

FIG. 5. Schematic showing a (010) section passing through a V_O center in a SrO plane in strained SrTiO_3 . In (a), the colors are as defined in Fig. 1, including the TiO_6 octahedra. In (b), the dashed circles show the unrelaxed sites of the oxygen ions in the TiO_2 , with the open and filled circles indicating oxygen and titanium atoms, respectively.

FIG. 6. Calculated inter-plane V_O migration barriers as a function of compressive strain for diffusion along Δ_{1-5} step (a, c, and e for neutral, +1, and +2, respectively) and Δ_{5-7} step (b, d, and f for neutral, +1, and +2, respectively), as shown in Fig. 3. Circles (red line) and squares (green line) refer to the forward and backward diffusion, respectively. The triangles (blue line) refer to the difference in the energy between the starting and the ending point of the diffusion.

difference between V_O in the TiO_2 and SrO planes is decreasing with increasing strain, leading to the reduction in total activation energy.

The greatest variation in the activation energy with charge state among the strains examined in this study appears at 6% strain, where the neutral oxygen vacancy migrates with a barrier around 0.1 eV lower than the ionized forms. In the neutral charge state, V_O has a deep double-donor level occupied by two electrons. When fully ionized, the absence of the two donor electrons leads to small changes in structure. We find that the differences are particularly noticeable at 6% strain. Consequently, the energy difference between the ending and the starting points for this step of diffusion is more dependent upon charge than for other mag-

nitudes of strain. We find that for the 6% case, the barriers are 0.68, 0.79, and 0.83 eV for the neutral, singly, and doubly ionized charge states, respectively.

2. The Δ_{5-7} step

As with the Δ_{1-5} step, the activation energies along the second stage, Δ_{5-7} , have been plotted, appearing in Figs. 6(b), 6(d), and 6(f) as a function of strain for neutral, +1, and +2, respectively. The clear trend is for the activation energy to increase with strain, with the effect so significant that at 6% the activation energy has more than doubled relative to the barrier in unstrained material. One reason for this dramatic increase is the same as in the first step: the distance required

FIG. 7. Side (top) and the perspective views (bottom) of V_O in different sites of compressively strained SrTiO_3 . (a) The vacancy within the TiO_2 plane, (b) the moving of the oxygen ion from the SrO plane to fill the vacancy (in TiO_2 plane) induced a migration of another oxygen ion to take a mid site between its original site and the vacancy, (c) the vacancy at the TiO_2 -plane which is equivalent to the vacancy in (a).

for the vacancy to move is increasing with increasing strain. However, in addition, as has been recently reported,⁵⁸ the rotation of the Ti 3d-orbitals due to the AFD reduces their overlap with oxygen 2p-orbitals within (001)-plane, while it is maintained along the [001]-direction.

IV. SUMMARY AND CONCLUSIONS

In summary, density functional calculations have been performed to ascertain the impact of interfacial (001) bi-axial compressive strain in SrTiO_3 upon the activation energy for diffusion of the electrically active oxygen vacancy, thought to be important in processes leading to electrical conduction (leakage current) in the use of SrTiO_3 as a dielectric material. It was found that this strain induces a combination of ferroelectric and antiferroelectric distortive modes of phase transition in the SrTiO_3 , with displacement of oxygen ions along the [001] direction relative to the metal ion sub-lattice, and rotation of the oxygen-octohedra about the same axis.

The impact upon diffusion is highly dependent both upon the magnitude of strain, and upon the direction of migration relative to the [001]-direction. Up to 50% reduction in the migration barrier has been found for in-plane migration, suggesting that such diffusion would increasingly occur at room temperature with increasing strain. In contrast, since the activation energy for diffusion in the direction normal to the plane of strain is dictated by the Δ_{5-7} step, the effect of isotropic bi-axial strain in the (001) plane is to significantly impede the diffusion in the direction normal to the plane of strain.

The barrier to injection of V_O into an epitaxial film is maximised, according to the current calculations, where the strain is in the vicinity of 6%, which represents the maximum in the activation energy calculated in this study. The magnitude of the barrier, being round 1.5 eV, is sufficiently large to significantly reduce diffusion at room temperature in

the absence of an applied electric field. Even at more modest strains, the impact of interfacial strain remains significant. At 2% strain, the in-plane diffusion remains approximately constant, but the inter-plane barrier has increased by about 35%–50% from 0.8 eV to around 1.1 eV with some variation with charge state.

In biased material, such as would be the case in capacitors or where SrTiO_3 is present as an epitaxial gate dielectric, there would be an effective reduction in the barrier for charged V_O , and an ion drift current may result in a thermal redistribution of these defects.

Nevertheless, the substantial diffusion anisotropy in compressively strained epitaxial material might be adopted as route to confine the diffusivity of these critically important electrically active defects. As such, strain may be viewed as a mechanism for the modification of leakage current in SrTiO_3 thin-films.

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