Effect of charge on point defect size misfits from ab initio: Aliovalently doped SrTiO₃

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Abstract

We demonstrate a computationally efficient method to calculate size misfits of point defects in aliovalently doped SrTiO₃ using density functional theory. The size misfits of neutral and charged single point defects are calculated and linearly combined to estimate the effective size misfits of multiple point defects in aliovalently doped SrTiO₃. The charge state has a demonstrable effect on point defect size misfits for both isolated and multiple defects. We attribute this to the different charge localization between the defective systems. The extra electron or hole for the charged isolated point defects compensates the difference of charge localization between the neutral point defects and aliovalently doped system. The sum of size misfits of charged isolated point defects accurately estimates size misfits for aliovalently doped SrTiO₃, without charge correction which was possibly required due to the additional charge state of point defect.

Keywords: size misfits, charged point defects, density functional theory, SrTiO₃

1. Introduction

The perovskite material strontium titanate (SrTiO₃) is used in a wide range of applications including buffer layers for epitaxial thin films, microwave resonators, and catalysts [1, 2, 3]. The dielectric properties of SrTiO₃ depend

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on its structural parameters such as lattice constants and the tolerance factor [4]. Many theoretical and empirical models predict the structural parameters based on the composition of perovskites [5, 6, 7]. However, these models do not account for the effects of dopants or vacancies on the structural parameters, despite the fact that SrTiO_3 is commonly doped by metals or trivalent rare earth elements to improve the dielectric properties [8]. Recently, Ubic *et al.* [9] controlled the Sr vacancy concentration in SrTiO_3 by doping with the trivalent atoms (La, Ce, and Nd), and measured the lattice constants according to the vacancy concentration. The authors suggest an improved empirical model to evaluate the pseudo-cubic lattice parameter and tolerance factor of aliovalently doped SrTiO_3 by accounting for the effective size of a vacancy at a Sr site.

Calculating formation volumes and energies of charged point defects using density functional theory (DFT) requires a careful approach to account for electrostatic interactions within the periodic cell and the potential shift [10, 11, 12]. In silicon, Bruneval *et al.* [13] described the potential bias caused by the charge state of point defects that significantly changes the formation volume and requires correction. They found that the corrected formation volume weakly depends on the defect type and charge state. Density functional theory studies of perovskites studies have focused on charged or neutral oxygen vacancies and their formation energies or electronic properties [14, 15], but not on formation volumes. The formation energy calculations for charged point defects require a charge correction to account for the potential shift in perovskites as well. These results suggest that the charge state could affect formation volume, and aliovalently-doped SrTiO_3 with experimentally measured lattice constants [9] provides an ideal system to answer this question. Aliovalently-doped SrTiO_3 contains two substitutional atoms (Ln_{Sr} , $\text{Ln} = \text{La, Nd, Ce}$) with a single vacancy (V_{Sr}) at Sr atomic sites given by

These trivalent substitutional elements have a +1 charge, compensated by the -2 charge of the Sr vacancy. Shanthi and Sarma computed charge distributions

in perfect SrTiO_3 and in neutral SrTiO_3 with a substitutional La solute on the Sr sublattice [16]. They find that the La does not yield midgap states, which is attributed to the La-derived electronic states occurring far below the Fermi energy. However, they didn't investigate the redistribution of charge in systems with multiple defects – i.e., aliovalently doped SrTiO_3 – or the effect of charge transfer on point defect size misfits.

We demonstrate a computationally efficient method to calculate the effective size misfits of point defects in aliovalently doped SrTiO_3 by linearly combining the size misfits of charged single point defects, without the need for charge correction. The size misfit calculation of single point defects produces a smaller finite size effect compared to the multiple defective geometry. We calculate the size misfits for multiple defects in aliovalently doped SrTiO_3 and single point defects for different charge states. The sum of size misfits of single charged defects *without correction* matches well with the size misfits of neutral defect complexes, while the sum of size misfits of single neutral defects disagrees. In addition, electrons and holes have different sizes in Sr vacancies compared with substitutional sites. We attribute the disagreement in size misfits to differences in charge transfer for neutral point defects compared with defect complexes in aliovalently doped SrTiO_3 .

2. Computational details

We perform DFT calculations using the Vienna ab-initio simulation package (VASP) [17, 18] based on plane wave basis sets. The projector-augmented wave (PAW) potentials generated by Kresse [19] describe the Sr ($[\text{Ni}]4s^24p^65s^2$), Ti ($[\text{Ne}]3p^63d^24s^2$), O ($[\text{He}]2s^22p^4$) and substitutional atoms (La, Ce, and Nd) with the same core electron configuration [Kr]. The Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA) functional [20] accounts for electron exchange-correlation energy. A plane-wave energy cutoff of 850 eV is required for an energy convergence of less than 1 meV/atom. A $2 \times 2 \times 2$ Monkhorst-Pack [21] k -point grid samples the Brillouin zone of the $3 \times 3 \times 3$ SrTiO_3 supercells (135

atoms). Gaussian smearing is employed for integrating the density of states with a smearing width of 0.05 eV. All the atoms in the supercells are relaxed until the force on each atom is less than 5 meV/Å. The SrTiO₃ unit cell has a cubic structure with computed lattice constant $a = 3.94$ Å and bulk modulus $B = 171.8$ GPa, which agree well with the experimental values of $a = 3.905$ Å [9] and $B = 174$ GPa [22]. It is assumed that the presence of defect does not change the bulk modulus significantly, thus negligible. We applied strain on unit cell from $\pm 0.1\%$ to $\pm 0.4\%$ by 0.1% difference to appropriate directions and relaxed ions with fixed volume to calculate three independent elastic constants C_{11} , C_{12} and C_{44} , where the calculated values are 320.3, 99.0 and 109 GPa respectively. Then, the bulk modulus B is calculated by $1/B = (S_{11}+S_{22}+S_{33})+2*(S_{12}+S_{13}+S_{23})$, where S_{ij} is the compliance tensor in Voigt notation which is the inverse of stiffness tensor. The calculated bulk modulus of SrTiO₃ using various exchange correlation functionals is compared [23], showing the range of bulk modulus from 159 to 222 GPa with different estimation of lattice constants. The electron density on each atomic site in the SrTiO₃ supercells is calculated using the Bader charge integration method [24].

The size misfit of a point defect is the fractional change of lattice constant a with respect to the concentration c of the defect. We compute size misfits ε_b by introducing point defects into a supercell and relaxing the atoms at fixed volume, which is found to be more suitable choice than the constant pressure method [10]. Point defects induce stress σ in the cell, which yields the size misfits as [25, 10]

$$\varepsilon_b = \left. \frac{1}{a} \frac{da}{dc} \right|_{c=0} \approx \frac{N\sigma}{3B}, \quad (2)$$

where N is the number of atoms in the supercell and B is the bulk modulus of undefective SrTiO₃. The size misfits of point defects in the aliovalently doped system are computed for $2 \times 2 \times 2$ and $3 \times 3 \times 3$ supercells to estimate finite size effects. The absolute errors for size misfit values between $2 \times 2 \times 2$ supercells and $3 \times 3 \times 3$ supercell are 0.010 and 0.038 for La and Ce, respectively. However, the Nd $2 \times 2 \times 2$ supercell calculations suffered from severe charge-sloshing

exacerbated by finite size effects. All reported size misfits are from the $3 \times 3 \times 3$ supercells.

3. Effective size misfits

Figure 1 shows the geometries used to calculate the size misfits of point defects in aliovalently doped systems using a direct method and an indirect method. The direct method calculates the size misfits using the SrTiO_3 structure containing two substitutional atoms and a Sr vacancy. In the direct method, the point defects are separated as far as possible from each other within the periodic geometry to minimize the effect of defect interactions on the size misfits. The absolute error of size misfits computed from two different atomic arrangements (i.e., different distances between point defects) using the $2 \times 2 \times 2$ supercell are 0.001 and 0.015 for La and Ce respectively, indicating that point defect interactions have a smaller effect than finite supercell size. The indirect method calculates the effective size misfits for the aliovalently doped systems by summing the size misfits of isolated neutral/charged point defects. This enables us to quantify the contribution of the point defect charge states to the effective size misfits.

Table 1: The size misfits (ε_b) of single point defects in the neutral (Ln_{Sr} or V_{Sr}) and the charged ($\text{Ln}_{\text{Sr}}^\bullet$ or V_{Sr}'') systems. The size misfit magnitudes and signs change when the point defects are charged: +1 for the substitutional atoms and -2 for the Sr vacancy.

	ε_b (neutral)	ε_b (charged)
La_{Sr}	0.0278	-0.230
Ce_{Sr}	-0.0102	-0.266
Nd_{Sr}	-0.0317	-0.284
V_{Sr}	-0.0652	0.317

Table 1 shows the strong dependence of size misfits on the charge state of single point defects in SrTiO_3 . The negative size misfits for neutral Ce, Nd, and

Figure 1: (color online). Geometry of SrTiO_3 (left) with two substitutional atoms ($\text{Ln}_{\text{Sr}} = \text{La, Ce, and Nd}$) and a Sr vacancy (V_{Sr}), and (right) with a single substitutional atom (Ln_{Sr}) or a Sr vacancy (V_{Sr}). The supercells without defects contain 27 Sr atoms (green), 27 Ti atoms (blue), and 81 O atoms (black).

vacancy indicate that the cell volume contracts when these defects are present in SrTiO_3 , while La causes the cell to expand. When the substitutional atoms are in a +1 charge state (i.e. addition of a hole) and the vacancy is in a -2 charge state (i.e. addition of two electrons), the magnitudes of the size misfits change by more than a factor of four. The addition of a hole for the substitutional atoms decreases the size misfits, whereas the addition of electrons for the Sr vacancy increase the size misfit from its value for the neutral state. This strong dependence of size misfits of isolated single point defects on the charge state causes the effective size misfit obtained through the indirect method to also depend on the charge state.

Table 2: Comparison of effective size misfits (ε_b) estimated from three different methods, followed by the size misfits difference (Diff.) which is an absolute error with respect to the direct method. The size misfits of point defects in aliovalently doped systems are directly computed from defective SrTiO_3 containing two substitutional atoms and a Sr vacancy, or indirectly by linearly combining the size misfits of the neutral/charged single point defects. Accounting for the charge states of the defects in indirect method decreases the size misfit difference with respect to direct method less than 10%.]

	Direct Method	Indirect method, Neutral		Indirect method, Charged	
	ε_b	$2\varepsilon_b(\text{Ln}_{\text{Sr}}) + \varepsilon_b(V_{\text{Sr}})$	Diff.	$2\varepsilon_b(\text{Ln}_{\text{Sr}}^{\bullet}) + \varepsilon_b(V_{\text{Sr}}'')$	Diff.
La_{Sr}	-0.131	-0.010	-0.121	-0.143	0.012
Ce_{Sr}	-0.199	-0.086	-0.113	-0.215	0.016
Nd_{Sr}	-0.237	-0.129	-0.108	-0.251	0.014

Table 2 shows that accounting for the charge states of isolated point defects reduces differences in the effective size misfits of point defects in aliovalently doped SrTiO_3 with respect to the direct method. The size misfits calculated using the direct method indicate that doping SrTiO_3 with different substitutional atoms contracts the lattice by different amounts. The effective size misfits computed indirectly from the size misfits of neutral single point defects have large differences compared to the values obtained using the direct method, while the

Figure 2: (color online). The size misfits (ε_b) of the substitutional atoms (Ln_{Sr}) and a vacancy (V_{Sr}) at a Sr site for different numbers of added/subtracted electrons. The size misfits vary linearly with similar slopes for substitutional atoms, whereas the linear variation for the Sr vacancy has a smaller slope. The slopes for La, Ce, Nd, and a vacancy are 0.258, 0.257, 0.255, and 0.190, respectively.

indirect method applied to *charged* single point defects reduces the differences by large amount. We note that the size misfit from indirect method by accounting for the charge state of single point defects agrees with the size misfit from direct method to within 10% without charge correction. The remaining size misfit differences are attributed to the different dependence of size misfit between the substitutional atoms and the vacancy on extra charge state of point defects.

The size misfits of charged point defects depend linearly on their charge state [13], and Figure 2 shows that the sizes of an extra electron and a hole are dependent on the defect type in SrTiO_3 . We interpret the size misfit change due to charge state of the defective system as the effective size of an extra electron or a hole. The linear change of size misfits with the addition of an electron or a hole indicates that the hole size is the negative of the electron size for each defect. However, the magnitude of the electron/hole size depends on point defect type. Thus, the size of the two electrons in the Sr vacancy does not cancel the size of the two holes for two substitutional defects. The different dependence of the

effective size of extra electron and hole on defect type is reflected in the charge distributions around the point defects in the neutral and charged systems.

4. Charge distribution

Figure 3 shows the difference in the charge distributions between two neutral single defects and aliovalently doped SrTiO_3 compared to defect-free SrTiO_3 . When La substitutes for a Sr atom, electrons localize around the La atom and more charge transfers to Ti atoms than other elements. When there is a Sr vacancy, the holes localize around the O atoms near the vacancy. For the aliovalently doped system, charge transfer occurs due to the presence of multiple defects within the system resulting in the smaller charge localization around the defects comparing to the single defective systems. The localized electron charges of the single neutral La substitutional atom and a neutral Sr vacancy (i.e. the sum of the electron charge of the nearest O atoms) with respect to the undefective cell are 0.51 and -0.75 . Within the aliovalently doped system, the localized charges of each La atom and a Sr vacancy with respect to the undefective cell are 0.48 and -0.59 . The redistribution of charge in aliovalently doped SrTiO_3 causes the different size misfits with respect to the indirect method applied on the neutral single defects.

Figure 4 shows that the extra hole and electrons introduced for charged single point defects are distributed throughout the supercell largely based on *chemistry*, not the distance from the defect. The extra hole for a La substitutional atom is distributed uniformly based on chemistry, with more transfer to Ti atoms than Sr, La, or O. For a Sr vacancy, the two extra electrons are mostly distributed on the O atoms and rest of the extra electrons in between zero to average value of extra electrons (i.e. $2/135$) distribute on the other atoms, but there are variations of magnitude for each atoms based on distance from the defect. This results in a small change in charge localization for the substitutional atom (-0.01) and a larger change for the Sr vacancy (0.23). The charged defects compensate the difference of charge transfer between the neutral single point

Figure 3: (color online). The difference in electron charge (Δn_e) at each atomic position between the neutral defective SrTiO_3 systems and undefective SrTiO_3 , with distance measured from the defect. The supercells contain a single La substitutional atom (top), a single Sr vacancy (bottom), and aliovalently doped SrTiO_3 with two La substitutional atoms and a Sr vacancy (middle). The distance is measured from the La atom (top) or the Sr vacancy position (bottom, middle). The Sr vacancy position is estimated by averaging the positions of its 12 oxygen nearest neighbors in the relaxed cell. The distribution of electron charge at each atomic position is calculated using Bader charge integration. The charge transfer occurs within multiple defects in aliovalently doped supercell, which explains the different magnitude of charge localization near point defects compared to the neutral isolated defect supercells.

Figure 4: (color online). The difference in electron charge (Δn_e) between the charged defective SrTiO₃ system and the neutral defective system, with distance measured from the defect. The supercells contain a single La substitutional atom (top) and a single vacancy (bottom) at a Sr site. The distance from the La substitutional atom or Sr vacancy is measured the same way as in Figure 3. The dashed lines show zero and the average electron density differences: $-1/135$ for $\text{La}_{\text{Sr}}^\bullet$ and $2/135$ for V_{Sr}'' . Both of an extra hole for the charged La substitutional atom and two extra electrons for charged Sr vacancy are not localized around defects, while showing different variations in spatial distribution.

defects and aliovalently doped system. The electron charges for the La substitutional atom and a Sr vacancy in the charged supercells are 0.50 and -0.52 , respectively, which are closer to the charge distribution of the aliovalently doped system. We observed the same trend for other substitutional atoms. A more accurate description of the charge distribution of the isolated defects produces better agreement with the size misfits of the complexes. Also, it suggests that the compensating background charge generated due to additional charge for charged point defect does not hinder the size misfit comparison between direct and indirect method.]]

Our work predicts the same trend of size misfits as experiment [9], with the largest value for La and the smallest value for Nd. The change of lattice parameter with Sr vacancy concentration is extracted from experimental data [9] to estimate the size misfits using Equation 2. The experimental size misfits of point defects in aliovalently doped SrTiO_3 are -0.023 , -0.030 , and -0.151 for La, Ce and Nd substitutional atoms, respectively. Interestingly, this trend relates to the effective ionic radii of substitutional atoms La, Ce and Nd, which are 103, 101 and 98.3 pm respectively [26]. The dopants with smaller ionic radii cause larger contraction of lattice, showing more negative value of size misfits for both of charged single substitutional atoms and aliovalently doped system. However, the magnitude of the experimental size misfits are smaller than what we find; it is possible this is due to multiple solute-solute, vacancy-vacancy and solute-vacancy interactions, as the experimental measurements include a much larger range of concentration than we consider here.

5. Conclusion

We describe a computationally efficient method to evaluate effective size misfits for aliovalently doped SrTiO_3 that linearly combines the size misfits of charged single point defects. We find that using defect size misfits extracted from charged supercells matches well with the effective size misfits directly computed from the aliovalently doped system. This is explained by the different electron

charge localization between the defective systems: the charge localization differences between the neutral single defects and the aliovalently doped system resulting from the charge transfer within multiple point defects, is compensated by the delocalized extra electron and hole distribution. We predict the same trend of size misfits as in experiments, the largest value for La and the smallest value for Nd, while the absolute values are larger than experimental values. The linear combination of isolated defect calculations enables us to account for the charge state of each single defect, and faster finite-size convergence than for multiple defective geometries. We expect this method to efficiently estimate the effective size misfits for multiple defects with different charge states within SrTiO₃ and other perovskite systems.

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