Nonlinear characteristics of structural properties and spontaneous polarization in wurtzite $Mg_xZn_{1-x}O$: A first-principles study

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First-principles calculations were carried out on the basis of the density functional theory to investigate the structural properties and spontaneous polarization in wurtzite $Mg_xZn_{1-x}O$. Random atomic configurations were applied to compute electronic ground states in large $4 \times 4 \times 3$ unit cells containing 192 atoms. Our theoretical calculation predicted a nonlinear characteristic of the lattice parameters a, c, and u of wurtzite $Mg_xZn_{1-x}O$, indicating the violation of Vegard's law. We also clarified a nonlinear characteristic of spontaneous polarization in the alloys and its almost linear dependence on the internal parameter u.

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I. INTRODUCTION

The group II oxides, such as MgO and ZnO, have attracted much attention as materials for optoelectronic devices, such as UV light emitting diodes, high-frequency and high-power electronic devices, transparent electronic devices, and piezoelectric devices, because the earth abundant and green characteristics of these oxides increase the importance as a material for these electronic devices. The large band gap of wurtzite $Mg_xZn_{1-x}O$ alloys ranging from 3.4 to about 7 eV leads to the development of ultraviolet light emitting diodes.[1–4] Similar to GaN/AlGaN,[5] a ZnO/MgZnO heterostructure is expected to exhibit the formation of a two-dimensional electron gas (2DEG),[6–8] which is necessary to fabricate a high electron mobility transistor (HEMT) without doping.

In order to design such devices, detailed information on fundamental physical and chemical quantities of wurtzite $Mg_xZn_{1-x}O$ is necessary in a wide range of x. However, those quantities are scarcely known, partly because the equilibrium structure of MgO is the rocksalt structure. Thus far, the structural properties of wurtzite $Mg_xZn_{1-x}O$ were investigated by Schleife *et al.*[9] and Fan *et al.*[10] by performing first-principles calculations, where the nonlinear characteristics were reported for the lattice parameters. In one of the reports,[9] the lattice parameter c and cation-cation distance d decrease with the increase in x. The decrease of cation-cation distance d implies the decrease of lattice constant a, conflicting with the experimental data of Ref. 11 suggesting the increase of a with the increase in x. The nonlinear characteristic of the lattice parameters was also reported by Park and Ahn,[12] introducing the experimental data of Makino *et al.*[13] and Ohtomo and Tsukazaki.[14] Experimental results at high Mg concentrations $x > 0.5$ of wurtzite $Mg_xZn_{1-x}O$ have scarcely been reported, because the cubic phase emerges at the large Mg mole fraction of $x > 0.53$.[15] Thus, the nonlinear characteristic of the lattice parameters should be investigated in detail especially for the large value of the Mg content x, because, in general, Vegard's law, which assumes linear relationship between the alloy composition and physical or chemical quantities, is used to predict those quantities of alloys.

Another conflict between the results of theories and an experiment has occurred about the value of the internal parameter u. Theoretical results[16–18] suggest that the u value of Mg-O bonds is larger than that of Zn-O bonds, while the experimental result by Kim *et al.*[19] indicates that the Mg atoms have a slightly reduced wurtzite parameter u and more regular tetrahedral bond distances than the Zn atoms.

Spontaneous polarization in wurtzite MgO and ZnO has been reported by only an experiment[12] and a few theoretical predictions.[17,20,21] Malashevich and Vanderbilt reported a first-principles investigation of the spontaneous polarization in wurtzite $Mg_xZn_{1-x}O$ in a range of $x < 0.5$ using 12 and 16 atoms in the unit cells, indicating a roughly linear dependence of spontaneous polarization on Mg concentration.[17] As the nonlinearity of the spontaneous polarization in group III-V nitride compounds has been reported by Bernardini and Fiorentini,[22] the similar nonlinear characteristic is also expected for that in wurtzite $Mg_xZn_{1-x}O$.

In this paper, we report on the computational results of the structural properties and spontaneous polarization in wurtzite $Mg_xZn_{1-x}O$ by means of the first-principles calculation on the basis of the density functional theory. The Mg mole fraction x is ranging from 0 to 1, and large $4 \times 4 \times 3$ unit cells are used to realize random atomic configurations to avoid compositional fluctuation in the unit cells.

II. COMPUTATIONAL METHOD

First-principles calculations were performed on the basis of the density functional theory[23] together with the generalized gradient approximation (GGA) for the exchange-correlation energy.[24] The projector augmented wave (PAW) pseudopotential method[25] was adopted to describe ion-electron interaction, and the nonlinear core correction[26] was applied to Mg, Zn, and O pseudopotentials. The Mg $3s^2$, Zn $3d^{10}4s^2$, and O $2s^22p^4$ electrons were included as valence electrons. Cutoff energies for plane-wave expansion were 40 and 240 Ry for a electronic wave function and charge density, respectively. Large $4 \times 4 \times 3$ unit cells of wurtzite $Mg_xZn_{1-x}O$ which contain 192 atoms were used to realize several mole fractions of x, where random atomic configurations were adopted in the unit cells to avoid compositional fluctuation. The random atomic configurations were determined such that each group II element has nearly the same number of elements around them in a certain radius. For each mole fraction, three different atomic configurations were prepared. Three atomic configurations of $Mg_{0.5}Zn_{0.5}O$ are shown in Fig. 1.

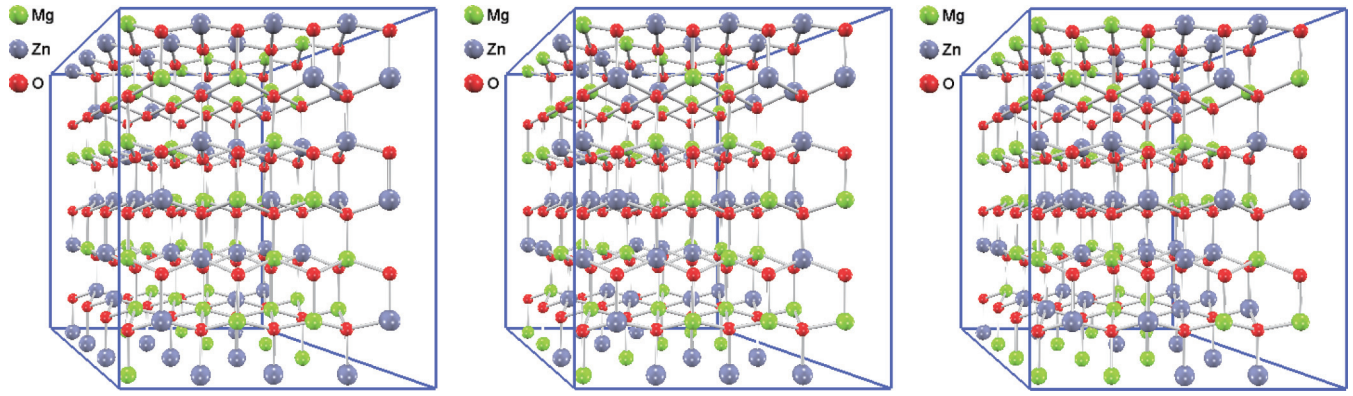

FIG. 1. (Color online) Three $4 \times 4 \times 3$ unit cells of wurtzite $Mg_{0.5}Zn_{0.5}O$ used in the computation. A random atomic configuration is applied so that the composition of every part in the unit cell is as uniform as possible.

The lattice parameters were fully optimized by minimizing the forces on atoms and stress tensors within 1×10^{-4} eV/Å and 0.05 GPa, respectively. The **k** point integration for computing electronic states was done by using a $2 \times 2 \times 2$ Monkhorst-Pack (MP) mesh,[27] and the polarization was computed by the geometric quantum phase (Berry phase) approach[28–30] using a $2 \times 2 \times 18$ MP mesh **k** point. Calculations in this paper were done by using the *ab initio* simulation package QUANTUM-ESPRESSO.[31]

III. RESULTS AND DISCUSSION

A. Structural properties

Our computational results of lattice parameters of MgO and ZnO are summarized in Table I together with the other theoretical and experimental data. The lattice constant a of the rocksalt structure of MgO is also listed. Our results are in good agreement with the experimental data and also with the theoretical prediction by Yan *et al.*[32] Excellent agreement of the lattice constant a of rocksalt MgO supports the reliability of our prediction of the lattice parameters of the wurtzite structure. The experimental values of wurtzite MgO were obtained by linear extrapolation of several experimental data of $Mg_xZn_{1-x}O$.[20] The nonlinear dependence of the lattice parameters on Mg concentration x, as will be described later, implies that the nonlinear extrapolation may give better agreement with our results. The theoretical prediction by Jang and Chichibu[20] slightly underestimates the lattice parameter a for both wurtzite MgO and ZnO even with the Hubbard U correction in conjunction with the local density approximation (LDA). Similarly, the LDA result of Malashevich and Vanderbilt[17] underestimates the lattice parameters of ZnO, where they have insisted that MgO has no stable wurtzite structure referring the same result by Limpijumnong and Lambrecht.[33] Further, the LDA result by Fan *et al.* also underestimates the lattice parameters a and c, while their internal parameter u is larger than the experimental result. To confirm the crystal stability of wurtzite MgO, we performed phonon calculations using both the GGA and LDA functionals. Both of the calculations resulted in no imaginary frequencies, and the wurtzite MgO structure was found to be one of the metastable structures in our calculation with the PAW pseudopotentials. The hexagonal MgO with the D_{6h}^4 symmetry is also the metastable structure having lower energy than the wurtzite phase, so that there is a possibility that $Mg_xZn_{1-x}O$ crystallizes in a hexagonal structure at high concentrations x.

TABLE I. Lattice parameters of MgO and ZnO.

		wurtzite			rocksalt
		a[nm]	c[nm]	u	a[nm]
MgO	Present	0.3289	0.5031	0.3952	0.4213
	Experiment	0.3283[a]	0.5095[a]	0.388[a]	0.4216[b]
	Theory[c]	0.3166	0.5070	0.380	
	Theory[d]	0.3278	0.5062	0.3919	
	Theory[e]	0.32786	0.48736	0.4046	
ZnO	Present	0.3253	0.5251	0.3790	
	Experiment[f]	0.3254	0.5206	0.380	
	Experiment[g]	0.3250	0.5210	0.3819	
	Theory[c]	0.3221	0.5040	0.386	
	Theory[d]	0.3264	0.5238	0.3807	
	Theory[e]	0.32032	0.51386	0.3814	
	Theory[h]	0.320	0.515	0.378	
	Theory[i]	0.3199	0.5167	0.379	

[a]Reference 20. Empirical linear least square fitting from experimental data of Refs. 11, 34–37.
[b]Reference 38, x-ray diffraction, powder samples.
[c]Reference 20, local density approximation (LDA) with Hubbard U correction.
[d]Reference 32, Heyd-Scuseria-Ernzerhof hybrid functional (HSE06).
[e]Reference 10, LDA with PAW pseudopotential.
[f]Reference 37, helicon-wave-excited-plasma sputtering epitaxy.
[g]Reference 19, x-ray diffraction, powder samples.
[h]Reference 21, LDA.
[i]Reference 17, LDA.

Figure 2 shows our computational results of the lattice parameters a and c in wurtzite $Mg_xZn_{1-x}O$. The value of the lattice parameter a is determined by averaging the two a values of the unit cell. In the supercell calculations, the crystal symmetry is not considered, so that the two a values are slightly different. The lattice parameters of our computational results show a nonlinear characteristic, indicating that the empirical Vegard's law does not hold.[9,12] The nonlinearity of the lattice parameters of wurtzite $Mg_xZn_{1-x}O$ are described as

$$a(x) = a_{\mathrm{MgO}}x + a_{\mathrm{ZnO}}(1-x) + b_a x(1-x) \qquad (1)$$

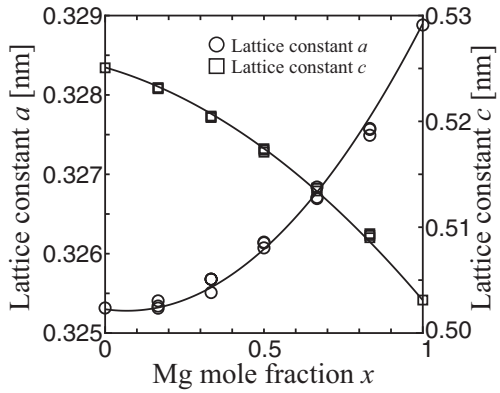

FIG. 2. Lattice constants a and c of wurtzite $Mg_xZn_{1-x}O$. Solid lines are the results of least square fits by Eqs. (1) and (2).

and

$$c(x) = c_{MgO}x + c_{ZnO}(1-x) + b_c x(1-x). \quad (2)$$

Nonlinear least square fits by Eqs. (1) and (2) to our results for the lattice parameters a and c generate $b_a = -0.004167$ nm and $b_c = 0.01333$ nm, where a_{MgO}, a_{ZnO}, c_{MgO}, and c_{ZnO} are fixed to our computational results of pure MgO and ZnO listed in Table I. The nonlinear characteristic of the lattice parameter a was also reported by Park and Ahn,[12] introducing the experimental data of Makino *et al.*[13] and Ohtomo and Tsukazaki.[14] In their report,[12] the bowing coefficient b_a is calculated to be -0.01097 nm, and the magnitude is larger than our result. The nonlinear characteristics of the lattice parameters are considered to originate from the difference in the chemical bonding property between MgO and ZnO, where the ionic MgO crystallizes in rocksalt, while ZnO forms the wurtzite crystal with covalent bonding.

Our computational result of the internal parameter u is shown in Fig. 3 as a function of the Mg mole fraction x. The plots are the averaged u values in the unit cells. The u values of Mg-O bonds are smaller than those of Zn-O, agreeing with the experimental result by Kim *et al.* where the range of the Mg mole fraction is $0 \leqslant x \leqslant 0.15$.[19] Another characteristic in the figure is a nonlinear dependence of the

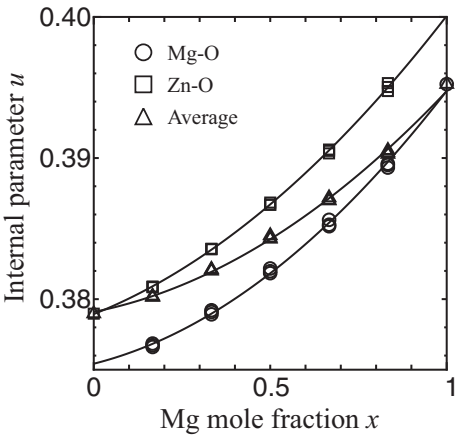

FIG. 3. Internal parameter u of wurtzite $Mg_xZn_{1-x}O$. Circles are the internal parameter u of Mg-O, squares are that of Zn-O, and triangles are the average of them.

TABLE II. Spontaneous polarization of wurtzite MgO and ZnO in units of C/m^2.

	MgO	ZnO
Present	−0.135	−0.034
Experiment[a]	−0.070	
Theory[b]	−0.080	−0.053
Theory[c]	−0.144	−0.022
Theory[d]	−0.111	−0.0322

[a]Reference 12, fitted by the non-Markovian gain model with many-body effects.
[b]Reference 20, LDA + U result.
[c]Reference 21. The value for MgO is calculated with the a parameter constrained to the ZnO experimental value (0.325 nm). The c/a and u parameters are relaxed.
[d]Reference 17. The value for MgO is obtained by the linear extrapolation of the computational data as shown in Fig. 4.

internal parameter u on x. This implies its correspondence to the nonlinear characteristic of the spontaneous polarization in wurtzite $Mg_xZn_{1-x}O$ as has been suggested in the case of nitride compounds.[22] The correlation between the values of spontaneous polarization and the internal parameter u will be described later.

B. Spontaneous polarization

The values of spontaneous polarization in wurtzite MgO and ZnO are summarized in Table II. The magnitude of spontaneous polarization of our MgO result is larger than the LDA + U result[20] and experimental data,[12] and is similar to one of the results of Gopal and Spaldin,[21] −0.144, which has been calculated at the a parameter constrained to the ZnO experimental value (0.325 nm) with the c and u parameters being relaxed. The linear least square fit to the theoretical prediction of Malashevich and Vanderbilt[17] also results in a large magnitude of spontaneous polarization of wurtzite MgO. The large difference between our result and the LDA + U result by Jang and Chichibu[20] is correlated to the difference in the predicted values of the internal parameter u. Another LDA result of ZnO by Malashevich and Vanderbilt[17] agrees with our result, because their u value is comparable to ours. This implies the prediction of the u value is significantly important for the accurate calculation of the value of spontaneous polarization in wurtzite alloys.

Figure 4 shows the computational result of the spontaneous polarization in wurtzite $Mg_xZn_{1-x}O$. First-principles prediction by Malashevich and Vanderbilt[17] is also shown by filled circles. The nonlinearity of the value of spontaneous polarization in wurtzite $Mg_xZn_{1-x}O$ can be described as

$$P(x) = P_{MgO}x + P_{ZnO}(1-x) + b_P x(1-x), \quad (3)$$

where P_{MgO} and P_{ZnO} are the values of spontaneous polarization of pure MgO and ZnO, respectively, and b_P is the bowing parameter. For further investigation of the nonlinearity of the spontaneous polarization in wurtzite $Mg_xZn_{1-x}O$, we divide the spontaneous polarization P into P_{id} and $P_{\Delta u}$, where P_{id} is the spontaneous polarization when u is the ideal value, 0.375, with the a and c parameters being fixed to the optimized values, and $P_{\Delta u}$ is the difference between P and P_{id}. Thus, $P_{\Delta u}$ is

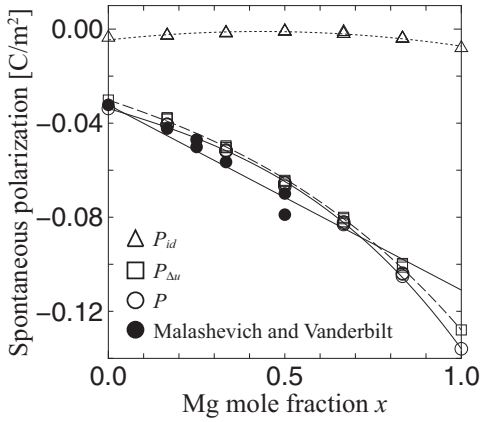

FIG. 4. Spontaneous polarization in wurtzite $Mg_xZn_{1-x}O$. Open circles are our result and filled circles indicate the theoretical result by Malashevich and Vanderbilt (Ref. 17). Solid and dashed curves are the results of least square fits by Eq. (5).

approximately expressed as

$$P_{\Delta u} = -\frac{NeZ^*c\Delta u}{V} = -\frac{NeZ^*\Delta u}{S}, \tag{4}$$

where N is the number of cations in the unit cell, e is the charge of an electron, Z^* is the averaged Born effective charge of cation, V is the volume of the unit cell, $S = V/c = \sqrt{3}a^2/2$, and Δu is the averaged difference of the internal parameter u from its ideal value of 0.375. If the value of $-NeZ^*/S$ is independent on u and thus on x, $P_{\Delta u}$ should be a linear function of u and thus a nonlinear quadratic function of x. The values of $-NeZ^*/S$ computed from $(P - P_{id})/\Delta u$ are shown in Fig. 5 as a function of both x and u. As shown in Fig. 5, the value of $-NeZ^*/S$ depends on x. Because of the scarce three samplings of the atomic configurations of each mole fraction, the dependence cannot be clearly determined whether it is linear or quadratic. Provided that $-NeZ^*/S$ is expressed by a linear function of x and considering the quadratic dependence of Δu on x, $P_{\Delta u}$ can be described as a cubic function of x. Since $P = P_{id} + P_{\Delta u}$, the spontaneous polarization P can also be described as a cubic function of x, where P_{id} also shows a

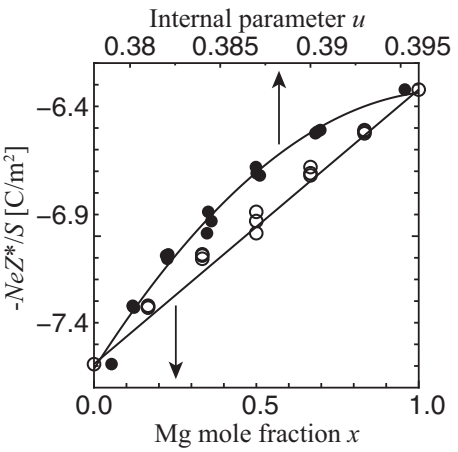

FIG. 5. The values of $-NeZ^*/S$ computed from $(P - P_{id})/\Delta u$. The open and filled circles are plotted as a function of x and u, respectively.

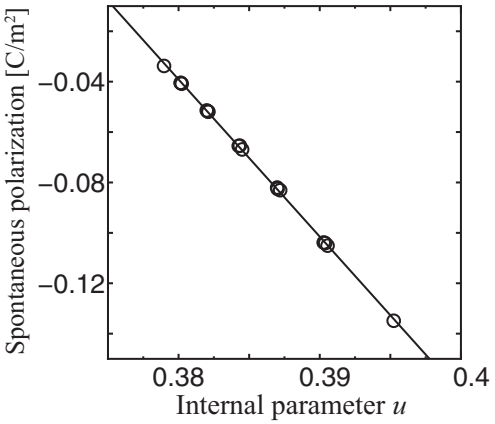

FIG. 6. Spontaneous polarization vs internal parameter u of wurtzite $Mg_xZn_{1-x}O$.

nonlinear quadratic dependence on x as can be seen in Fig. 4. The cubic dependence of the spontaneous polarization P on x thus can be expressed as

$$P(x) = P_{\mathrm{ZnO}} + x[(P_{\mathrm{MgO}} - P_{\mathrm{ZnO}})x + b_1(1-x) + b_2x(1-x)]. \tag{5}$$

A least square fit results in $b_1 = -0.0450$ C/m^2 and $b_2 = 0.0461$ C/m^2. Malashevich and Vanderbilt reported a roughly linear dependence of spontaneous polarization on Mg concentration.[17] The linear least square fit to their result gives $P_{\mathrm{MgO}} = -0.111$ C/m^2, which is slightly smaller than our value, where the value of P_{ZnO} is fixed to that of pure ZnO, -0.0322 C/m^2.

Figure 6 shows the correlation between the internal parameter u and spontaneous polarization in wurtzite $Mg_xZn_{1-x}O$. As shown in Fig. 5, $-NeZ^*/S$ has a nonlinear dependence on u, so that the spontaneous polarization should not show a clear linear dependence on u. However, it seems that an almost linear dependence on the internal parameter u because of the small change in $-NeZ^*/S$ in a narrow range of u.

IV. SUMMARY

We performed first-principles calculations to investigate structural properties and spontaneous polarization in wurtzite $Mg_xZn_{1-x}O$, applying random atomic configurations in large $4 \times 4 \times 3$ unit cells containing 192 atoms to avoid compositional fluctuation. We found a nonlinear characteristic for both of them in a wide range of x, indicating the violation of the empirical Vegard's law. We also clarified the correspondence between the nonlinear characteristics of spontaneous polarization and the internal parameter u in the alloy.

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