Effect of Interionic Interaction on the Electronic Polarizability, Optical Basicity and Binding Energy of Simple Oxides

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単純酸化物の電子分極率，光学的塩基度及び結合エネルギーに対するイオン間相互作用の効果

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Interaction parameter A proposed in Yamashita-Kurosawa's theory has been calculated for numerous single component oxides. It has been assumed that in the case of simple oxides it represents, through the electronic polarizabilities of the ionic pair the interaction between oxide ion and the corresponding cation due to overlapping of their outermost electronic orbitals to form a chemical bond. It has been proposed that the parameter A is closely related to the polarizability of the oxide ion as well as the optical basicity of the oxides. The obtained almost linear distribution of the basicity in respect to Yamashita-Kurosawa's parameter A could be used as an optical basicity scale for simple oxides. Systematic decrease of the O1s and outermost cation binding energies with decreasing interaction parameter has been established. It has been associated with decreased charge overlapping between electronic shells of the oxide ion and cation, which relates to large electronic polarizabilities of both cation and oxide ion and increased optical basicity, that is increased ionicity of the chemical bond.

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1. Introduction

Yamashita and Kurosawa^{1,2)} have proposed a general theory of the dielectric constant of simple ionic crystals based on quantum-mechanical treatment of the electronic structure of constituent ions in order to take into account the effect of charge overlapping between neighboring ions. In that theory the perturbed wave function of 2p electrons of a negative ion such as F^- and O^{2-} was used. The total energy change of the crystal due to the applied electric field was expressed by sum of three components:

$$\Delta E = \Delta E_0 + \Delta E_1 + \Delta E_2 \quad (1)$$

where ΔE_0 is the energy change of the positive and negative ions in free state, ΔE_1 the change of the electrostatic mutual interaction energy between them and ΔE_2 the change of the exchange energy between the ions. The simplest model of such energy change is polarization of ionic pair in high frequency field neglecting the polarization of the positive ion. In that case the quantum mechanical equation describing ΔE contains terms assigned to the energy changes ΔE_1 and ΔE_2 due to the possible interionic interaction of a negative ion only with its nearest neighbors. According to Yamashita and Kurosawa^{1,2)} a quantitative measure of this complex interaction is given by the so-called interaction parameter A , which in fact for a chosen cation-anion pair represents the charge overlapping of the negative ion with its nearest positive neighbor. By this manner it correlates with reducing the polarizability of negative ion placed in crystal lattice in respect to the free-ion polarizability.

Dikshit and Kumar³⁾ have suggested a simple way for evaluation of the interaction parameter A , based on Yamashita-Kurosawa's theory. They have calculated A for large number halide crystals as well as for four alkaline-earth oxides MgO, CaO, SrO and BaO, respectively. It was established that interaction parameter A decreases in the sequence $MgO \rightarrow CaO \rightarrow SrO \rightarrow BaO$.

In our recent paper the electronic polarizability of oxide ion $\alpha_{O^{2-}}$ and optical basicity A of numerous single component oxides including alkaline-earth oxides were estimated

on the basis of their refractive index and energy gap, respectively.⁴⁾ It was established also that O1s binding energy in the simple oxides decreases with increasing oxide ion polarizability, cation polarizability and optical basicity.⁵⁾ Simultaneously a decrease of metal (or nonmetal) binding energy in XPS spectra of simple oxides takes place with decreasing of O1s binding energy that is related to increased basicity. Interaction between O2p and outermost cation orbitals was assumed.⁶⁾ In this connection it is of interest to notice that a good correlation could be found between observed trend of the interaction parameter A established by Dikshit and Kumar³⁾ in the $MgO \rightarrow CaO \rightarrow SrO \rightarrow BaO$ series and the change of the oxide ion polarizability, optical basicity and binding energies of the same oxides found by us.⁴⁻⁶⁾ In short, the electronic polarizability of oxide ion and optical basicity increase while O1s and metal binding energies decrease in the pointed sequence of oxides. On this basis it seems that the interaction parameter A could be used probably as a quantity directly related to the chemical bonding in oxide materials. With a view to elucidate the chemical origin of the interaction parameter, in this paper, we continued the investigation on the polarizability in oxide systems searching for suitable relationships between electronic polarizability, optical basicity and binding energies and interaction parameter between ions proposed by Yamashita and Kurosawa in a large number of simple oxides.

2. Results

2.1 Calculation of interaction parameter in simple oxides

The analysis performed by Dikshit and Kumar³⁾ on the basis of the theory proposed by Yamashita and Kurosawa^{1,2)} allows to derive the following expression for calculation of the interaction parameter A for a given cation-anion pair,

$$A = \frac{[(\alpha_i^+ + \alpha_f^-) - (\alpha_c^+ + \alpha_c^-)]}{2(\alpha_i^+ + \alpha_f^-)(\alpha_c^+ + \alpha_c^-)} \quad (2)$$

where α_i^+ and α_f^- are the electronic polarizabilities of the

positive and negative ions in free-state, while α_c^+ and α_c^- are the electronic polarizabilities of the ions in crystal under consideration.

The most familiar and widely used relationship for estimation of the molar electronic polarizability of a given substance is the Lorentz-Lorenz equation. Generally, the application of that equation allows determination of the oxide ion polarizability of the material under consideration by subtracting its cation polarizability from the molar polarizability. This approach has been introduced mainly for crystalline and vitreous silicates starting by pioneering works by Kordes,⁷⁾ Fajans and Kreidl⁸⁾, and Weyl and Marboe.⁹⁾ Later it has been performed by Duffy¹⁰⁾ for several oxides and by Iwamoto et al.^{11),12)} and Duffy¹³⁾ for some silicate glasses. Recently, Dimitrov and Sakka⁴⁾ calculated by means of the Lorentz-Lorenz equation the electronic polarizability of oxide ion ($\alpha_{O^{2-}}$) of large number of simple oxides on the basis of two independent initial values: linear refractive index (n_o) and energy gap (E_g). The simple oxides have been classified in three groups on the basis of the average electronic polarizabilities of the oxide ion:⁴⁾ (a) oxides with polarizability between 1 and $2\text{\AA}^3$; (b) oxides with polarizability between 2 and $3\text{\AA}^3$; and (c) oxides with polarizability above $3\text{\AA}^3$. For the estimation of the polarizability of the oxide ion the values of free-cation polarizability proposed by Kordes¹⁴⁾ were used,⁴⁾ excepting these for Mn^{2+} , Fe^{3+} , Co^{2+} , Ni^{2+} , Cu^{2+} , Sb^{3+} , Te^{4+} , and Bi^{3+} which were taken from Refs. 15)–18). The values of oxide ion polarizabilities $\alpha_{O^{2-}}$ as well as the free-cation polarizability values used for their evaluation are presented in Table 1 (columns 2 and 3). We used here oxide ion

polarizability $\alpha_{O^{2-}}$ calculated as a mean value between refractive index $\alpha_{O^{2-}}(n_o)$ and energy gap $\alpha_{O^{2-}}(E_g)$ based oxide ion polarizabilities given in Ref. 4) because a good agreement exists between them. The data of the polarizability of oxide ion in BeO , P_2O_5 and Al_2O_3 are taken from Refs. 19) and 20). Recently, the approach proposed for simple oxides⁴⁾ was successfully extended by Vithal et al.²¹⁾ and Dimitrov and Komatsu²²⁾ for different binary oxide glasses.

As was discussed above the use of the Lorentz-Lorenz equation for determination of the oxide ion polarizability in general is connected with subtraction of the free-cation polarizability from the experimental molar polarizability. The subtraction is reasonable because the deformability of the electron cloud of the oxide ion is significant larger than that of the cations. Even though large size, a cation is not likely to be particularly polarized because the cationic charge will tend to hold on to the cationic electrons.²³⁾ On this basis assuming that the polarizabilities of the cations in the simple oxides are very close to their free-ion values we can modify Eq. (2) using the approximation $\alpha_c^+ \approx \alpha_f^+$. For metal (or nonmetal)-oxygen ionic pair after substitution also of α_c^- by $\alpha_{O^{2-}}$ this assumption leads to:

$$A = [(\alpha_f^- - \alpha_{O^{2-}})]/2(\alpha_f^+ + \alpha_f^-)(\alpha_f^+ + \alpha_{O^{2-}}) \quad (3)$$

where now α_f^- is the electronic polarizability of free oxide ion and $\alpha_{O^{2-}}$ is its polarizability in the crystalline oxide under consideration. We have calculated interaction parameter A for numerous simple oxides using Eq. (3) on the basis of the polarizability data of oxide ions and cations collected in Table 1 (columns 2 and 3). Pauling's value of $3.921\text{\AA}^3$ for the electronic polarizability of free oxide ion is used.²⁴⁾ The results are given in Table 1 (column 4).

Table 1. Oxides, Polarizability of Oxide Ion $\alpha_{O^{2-}}$, Free-Cation Polarizability α_f^+ , Interaction Parameter A , Optical Basicity Λ , OIs Binding Energy E_b , Element Binding Energy E_B^e and Cation Binding Energy in Oxides E_B^c

Oxide	$\alpha_{O^{2-}}$ $\text{\AA}^3$	α_f^+ $\text{\AA}^3$	A $\text{\AA}^{-3}$	Λ	E_b eV	E_B^e eV	E_B^c eV
Li_2O	2.090	0.024	0.110	0.87	-	56	-
BeO	1.290	0.007	0.258	0.375	-	113	113.5
B_2O_3	1.345	0.002	0.244	0.425	533.2	191	193.1
MgO	1.687	0.094	0.156	0.68	530.9	51	52.2
Al_2O_3	1.460	0.054	0.204	0.60	531.2	74	74.7
SiO_2	1.427	0.033	0.216	0.50	532.8	102	103.4
P_2O_5	1.350	0.021	0.238	0.33	533.5	133	135.0
CaO	2.420	0.469	0.059	0.975	529.8	25	-
Sc_2O_3	2.075	0.287	0.093	0.87	-	31	-
TiO_2	2.278	0.184	0.081	0.97	529.7	37	-
V_2O_5	2.643	0.122	0.057	1.04	530.0	40	42.1
MnO	2.330	0.544	0.062	0.95	529.8	-	-
Fe_2O_3	2.557	0.437	0.052	1.02	530.0	-	-
CoO	2.405	0.508	0.059	0.98	529.9	-	-
NiO	2.210	0.266	0.083	0.915	530.0	-	-
CuO	2.900	0.437	0.035	1.10	530.3	-	-
ZnO	2.859	0.283	0.040	1.08	530.3	10	10.04
Ga_2O_3	1.822	0.195	0.126	0.755	530.6	20	20.3
GeO_2	1.720	0.137	0.146	0.70	531.3	31	32.5
SrO	3.150	0.861	0.020	1.14	529.0	20	-
Y_2O_3	2.458	0.544	0.055	0.99	529.3	25	-
ZrO_2	1.975	0.357	0.097	0.825	529.9	29	-
Nb_2O_5	2.679	0.242	0.051	1.05	-	35	40.8
MoO_3	2.769	0.169	0.048	1.07	530.4	38	-
CdO	2.993	1.054	0.023	1.115	528.6	11	12.2
In_2O_3	2.762	0.662	0.037	1.07	530.1	19	18.0
SnO_2	2.050	0.479	0.084	0.85	530.1	25	-
Sb_2O_3	3.429	1.111	0.011	1.18	-	-	-
TeO_2	2.401	1.595	0.034	0.975	530.5	14	12.0
BaO	3.741	1.595	0.003	1.22	528.2	-	13.5
CeO_2	2.522	0.702	0.047	1.01	529.1	18	-
Ta_2O_5	2.291	0.185	0.080	0.94	-	25	26.4
WO_3	2.670	0.147	0.055	1.045	530.2	34	35.6
PbO	3.381	3.623	0.005	1.18	529.7	-	-
Bi_2O_3	3.507	1.508	0.008	1.19	-	-	-

2.2 Dependence of oxide ion polarizability on the interaction parameter

We have plotted the data of polarizability of oxide ion in simple oxides $\alpha_{O^{2-}}$ as a function of interaction parameter A in Fig. 1. A pretty good gradual trend of increasing the polarizability of oxide ion with decreasing interaction parameter can be observed. This result is in agreement with Yamashita-Kurosawa's theory^{1,2)} and shows that large value of A corresponds to low polarizability of the negative ion and vice versa. Simultaneously, a good correlation can be found between the oxide distribution in Fig. 1 and classification of simple oxides on the basis of their polarizability proposed by Dimitrov and Sakka.⁴⁾ Oxides such as BeO, B₂O₃, SiO₂, Al₂O₃, MgO, GeO₂, Ga₂O₃ show the largest interaction parameter in the 0.1–0.3 Å⁻³ range. The most transition oxides as well as oxides as SnO₂, CaO, TeO₂ and In₂O₃ possess intermediate interaction parameter between 0.03 and 0.1 Å⁻³ approximately. The lowest value of interaction parameter below 0.03 approximately present oxides such as CdO, SrO, PbO, Sb₂O₃, Bi₂O₃ and BaO.

2.3 Dependence of optical basicity on the interaction parameter

The intrinsic relationship between the oxide ion polarizability and the optical basicity of the medium has been shown by Duffy and Ingram^{25,26)} in terms of Jorgensen's h functions:

$$A = h'/h \quad (4)$$

where h and h' are related to a single monoatomic ion in its unpolarized and polarized states. They have proposed optical basicity as a measure of the acid–base properties of the oxides and glasses. For oxide material the Jorgensen h function indicates electron donor power of the oxide ion and shows that the ability to transfer electrons to surrounding cations depends from the degree of its polarization.

Dimitrov and Sakka⁴⁾ have estimated using the approach proposed by Duffy¹⁰⁾ the optical basicity of numerous simple oxides on the basis of average oxide ion polarizability calculated from the refractive index and the energy gap. A good agreement was observed between the optical basicity data obtained using independent initial quantities and these

obtained by Duffy. The optical basicity data A are presented in Table 1 (column 5), which are derived from refractive index and energy gap. The data for P₂O₅ and Al₂O₃ are according to Duffy.²⁰⁾ Optical basicity of BeO (0.375) was calculated in the present paper using the approach proposed in Refs. 4) and 10) taking into account the data for oxide ion polarizability (1.290 Å³) reported by Tessman et al.¹⁹⁾ On the basis of the similarity in the physical nature of the optical basicity and oxide ion polarizability we have plotted the data on the optical basicity against the data of interaction parameter in Fig. 2. As can be seen the optical basicity increases almost linearly with decreasing interaction parameter. The more acidic oxides such as P₂O₅, B₂O₃, SiO₂ and Al₂O₃ possess large interaction parameter, while more basic oxides for example CdO, SrO, PbO, Sb₂O₃, Bi₂O₃ and BaO show the lowest values of the interaction parameter. The most transition oxides as well as SnO₂, CaO, TeO₂ and In₂O₃ demonstrate intermediate values.

2.4 Dependence of O1s binding energy on the interaction parameter

Recently, Barr²⁷⁾ has reported comprehensive data on the O1s peak position in XPS spectra of large number of simple oxides. It was established that O1s binding energy of different oxides varies in 528.0–533.5 eV range. The O1s chemical shift corresponds to the different degree of ionicity in the M–O bonds. The simple oxides have been separated in three groups: (a) semicovalent oxides with O1s binding energy in 530.5–533.0 eV range; (b) normal ionic oxides with O1s binding energy at 530 ± 0.4 eV; and (c) very ionic oxides with O1s binding energy in 529.5–528.0 eV range.

Since both O1s binding energy and interaction parameter are two different physical properties of the oxide ion, it is of interest to check the correlation between them. For this purpose in Table 1 (column 6) O1s binding energies of various single component oxides are collected. The presented data are mainly according to Barr²⁷⁾ excepting these for TeO₂, B₂O₃, PbO and P₂O₅, which are taken from Refs. 28)–31), respectively. These data are plotted as a function of the

Fig. 1. Oxide ion polarizability $\alpha_{O^{2-}}$ as a function of interaction parameter A .

Fig. 2. Optical basicity Δ as a function of interaction parameter A . Fig. 3. O1s binding energy E_b as a function of interaction parameter A .

calculated data for interaction parameter in Fig. 3. There is a general trend of decrease of O1s binding energy with decreasing interaction parameter. At the same time good correlation can be found in the distribution of the simple oxides in Fig. 3 and classification of simple oxides proposed by Barr.²⁷⁾ It is seen that P_2O_5 , B_2O_3 , SiO_2 , Al_2O_3 , MgO , GeO_2 and Ga_2O_3 with high interaction parameter possess high binding energy in 530.5–533.0 eV range. These are more covalent oxides. The most transition oxides as well as SnO_2 , CaO , TeO_2 and In_2O_3 have O1s binding energy in narrow range at 530 ± 0.5 eV and intermediate interaction

parameter. These oxides belong to the normal ionic oxides. A few oxides, CeO_2 , SrO , CdO and BaO , show the lowest binding energy in 529.5–528.0 eV range and the lowest interaction parameter. According to Barr²⁷⁾ they represent the group of very ionic oxides.

2.5 Dependence of metal (or nonmetal) binding energy on the interaction parameter

Recently, Dimitrov and Komatsu⁶⁾ have demonstrated the intrinsic relation between O1s binding energy and metal (or nonmetal) binding energy obtained from XPS spectra for a numerous simple oxides. The term “metal (or

Fig. 4. Metal (or nonmetal) binding energy E_B as a function of interaction parameter A ($\circ$ element binding energy, $\bullet$ cation binding energy in oxides).

nonmetal) binding energy (E_B)” was introduced to denote both: binding energy of the outermost orbital of a cation in an oxide (E_B^c) as well as the binding energy of the same orbital in the corresponding pure element (E_B^e). It was established that high O1s binding energy correlates with high metal (or nonmetal) binding energy and vice versa. On this basis in the present paper we have searched for reasonable relationship between metal (or nonmetal) binding energy and interaction parameter of the oxides. For this purpose the element (E_B^e) and cation (E_B^c) binding energies are collected in Table 1 (columns 7 and 8). The element binding energies are taken from Briggs and Seah³²⁾ and these for cations in real oxides are taken from Ref. 33) excepting for those of V_2O_5 , In_2O_3 , BaO and TeO_2 which are according to Refs. 34)–37). The literature data of the metal (or nonmetal) binding energy as a function of the calculated values of interaction parameter are plotted in Fig. 4. As can be seen in general metal (or nonmetal) binding energy decreases from B_2O_3 to BaO with decreasing interaction parameter.

3. Discussion

The obtained results show that probably intrinsic relationships are found between interaction parameter A proposed by Yamashita and Kurosawa^{1,2)} and the observed trend in the electronic polarizability of oxide ion, optical basicity and binding energies in series of simple oxides. The results are good ground for discussing on the meaning of this physical constant derived now for a numerous simple oxides with a view to its practical use in the field of chemistry and materials science. Such discussion is necessary because the simple oxides are usually initial components for synthesis of different crystalline and amorphous materials.

The physical meaning of the interaction parameter A proposed by Yamashita and Kurosawa relates to the charge overlapping between neighboring ions. It has been introduced on the basis of quantum mechanical treatment of 2p-electron configuration of the negative ion. Therefore, in the case of simple oxides it represents the interaction of the ox-

ide ion with neighboring cation due to the charge overlapping. From chemical point of view such overlapping arises in chemical bonding. According to the fundamental theory³⁸⁾ the formation of the chemical bond between two ions or atoms is the result of overlapping of their outermost electron clouds. In the case of simple oxides the bonding realizes due to the interaction between 2p electrons of the oxide ions and outermost valence electrons of the cation. The product of that interaction is ionic-covalent chemical bond. Therefore, the observed similarity in two approaches probably is prerequisite for the correlation observed in Figs. 1–4. As can be seen from Eqs. (2) and (3) the interaction parameter is sensitive to the changes in the electronic polarizabilities of the oxide ion and cation. In our previous article⁵⁾ it was found that the polarizability of oxide ion and the optical basicity of simple oxides relate to O1s binding energy derived from XPS spectra. The observed chemical shift from 533.5 to 528.2 eV of O1s peak was explained with an increase in electron charge density of the oxide ions due to an increase in their electronic polarizability. At the same time increased polarizability of the oxide ion means stronger electron donor ability of the oxide ions corresponding to increased basicity. On the basis of the agreement found between the classifications of simple oxides made by Dimitrov and Sakka⁴⁾ and by Barr,²⁷⁾ the authors⁵⁾ separate oxides into three groups: (a) oxides such as P_2O_5 , SiO_2 , Al_2O_3 , GeO_2 , Ga_2O_3 with low oxide polarizability between 1 and $2\text{\AA}^3$, high O1s binding energy between 533.5 and 530.5 eV and relatively low optical basicity; (b) some main group oxides such as CaO , In_2O_3 , SnO_2 and TeO_2 as well as the most transition metal oxides with oxide polarizability between 2 and $3\text{\AA}^3$, O1s binding energy in very narrow range between 530.5–529.5 eV approximately and optical basicity close to that of CaO ; (c) a few oxides such as CdO , SrO and BaO with oxide ion polarizability above $3\text{\AA}^3$, the lowest values of O1s binding energy below 529.5 eV and optical basicity higher than that of CaO . That classification is in agreement with previously reported by Miura and Nanba³⁹⁾ basicity scale based on O1s

chemical shift in XPS spectra of a number of oxide glasses.

Simultaneously, it is necessary to notice that the distribution of the simple oxides observed in the Figs. 1–3 in respect to the interaction parameter is in good agreement with the classifications of simple oxides discussed above.^{4),5),27)} Generally, semicovalent oxides such as BeO, B₂O₃, SiO₂, Al₂O₃, MgO, GeO₂ and Ga₂O₃ with O1s binding energy in 530.5–533.0 eV range, oxide ion polarizability between 1 and 2 Å³ and low optical basicity show the largest interaction parameter. The normal ionic oxides such as transition oxides as well as SnO₂, CaO, TeO₂ and In₂O₃ with O1s binding energy at 530 ± 0.5 eV, polarizability of the oxide ion between 2 and 3 Å³ and optical basicity close to that of CaO possess an intermediate interaction parameter. The very ionic oxides such as CdO, SrO and BaO as well as PbO, Sb₂O₃ and Bi₂O₃, with O1s binding energy in 529.5–528.0 eV range, polarizability of oxide ion above 3 Å³ present the lowest value of the interaction parameter. In short, the observed increase in polarizability of the oxide ion as well as optical basicity and decrease in O1s binding energy of simple oxides (Figs. 1–3) could be explained with decreased interaction inside the ionic pair resulting in smaller overlap between O2p and cation valence orbitals. In result the amount of the unshared 2p-electron density available for donation of the average oxide ion increases. Therefore, it seems reasonable to assume an obvious correlation between parameter *A* and the relative amount of that density.

In this connection Dimitrov and Komatsu⁶⁾ have established that the increase of the polarizability of the oxide ion and the optical basicity of simple oxides is accompanied by decreasing metal (or nonmetal) binding energy. It was proposed that metal binding energy could be used as a measure of cation polarizability. It is of interest that the mentioned binding energies are the outermost energies near the valence levels. According to Barr and Brundle³⁶⁾ interaction works between outermost cation and oxygen 2p band. The interaction is responsible for the larger shift of O2p band to the Fermi level, and it is significant for cations with low-lying outermost levels. The shift of the O2p band is accompanied with moving down of all other oxygen dominated 2s and 1s levels. In other words the oxygen becomes more negative. According to Barr²⁷⁾ a shift of the leading edge of O2p dominated valence band in the XPS spectra of simple oxides toward the pseudo-Fermi level is a direct measurement of increased ionicity. As can be seen oxides such as BaO, CdO, SrO, TeO₂, In₂O₃, ZnO and CeO₂ (Fig. 4, Table 1) with low-lying outermost cation orbitals possess the lowest interaction parameter *A* below 0.05. This means decreased charge overlapping between valence electronic shells of the oxide ion and cation, which relate to large electronic polarizability of both cation and oxide ion and increased optical basicity, that is, increased ionicity. By contrast, oxides such as B₂O₃, P₂O₅, BeO, SiO₂ and Al₂O₃ with high-lying outermost cation orbitals possess the largest interaction parameter *A*, which indicates large overlapping of the valence electronic shells. Their polarizability of both oxide ion and cation is low, which is accompanied with low optical basicity and increased covalency. In this connection detailed and systematic investigations of the valence band spectra of different crystals and glasses including simple oxides would give a remarkable information about the origin of the chemical bonding and related polarizability phenomena. The recent studies concerning molecular orbital calculation and experimental valence band spectra in tellurite and borate crystals and glasses are good contribution in this field.^{40),37),41)–43)}

Briefly, the proposed by Yamashita and Kurosawa^{1),2)} interaction parameter *A* in the case of simple oxides represents the state of polarization of the average oxide ion.

It is the result of interaction between 2p-electron cloud of the oxide ion and valence cloud of the cation in respect to form a chemical bond. By this manner it seems that the interaction parameter *A* probably correlates with the unshared 2p electron density at average oxide ion available for donation. Low interaction parameter means large unshared 2p-electron density and vice versa. On this basis the obtained almost linear relationship between optical basicity, as a property closely related to the polarizability of the oxide ion, and the interaction parameter shows that parameter *A* could be used as a representative quantity for estimation and prediction of the basicity in different crystalline and amorphous materials.

4. Conclusion

The interaction parameter *A* introduced by Yamashita and Kurosawa for describing the dielectric properties of ionic crystals was calculated for a large number of simple oxides using the approach proposed by Dikshit and Kumar. The relationships between polarizability of the oxide ion, optical basicity, O1s binding energy and metal binding energy as a function of the interaction parameter were investigated. It was found that in the case of simple oxides the interaction parameter represents the polarizability state of the average oxide ion and its ability to form ionic-covalent bond with the cation. It was proposed that interaction parameter *A* is in agreement with previously reported simple oxide classifications and could be used as a representative quantity of optical basicity in simple oxides.

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