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# Elastic properties of $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$ phases ( $n = 1-3, \infty$ )

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## Abstract

Using *ab initio* calculations, we have studied the correlation between the electronic structure and elastic properties of  $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$  (space groups  $Pm\bar{3}m$  and  $I4/mmm$ ;  $n = 1-3, \infty$ ). These ternary oxides possess an unusually large bulk modulus to  $C_{44}$  ratio and the Peierls stress is comparably low. This may be understood on the basis of the electronic structure: ionic-covalent layers (Ti–O) are interleaved with metallic layers (Ti–Sr and Ti–Ti). We suggest that the large bulk modulus to  $C_{44}$  ratio and low Peierls stress are the result of weak coupling between the ionic-covalent and metallic layers, causing the low  $C_{44}$  value, as well as strong coupling within ionic-covalent layers, causing the large bulk modulus.

(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

For  $n = \infty$  the series of  $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$  converges to  $\text{SrTiO}_3$  (space group  $Pm\bar{3}m$ ). For  $n = 1-3$   $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$  yields  $\text{Sr}_2\text{TiO}_4$ ,  $\text{Sr}_3\text{Ti}_2\text{O}_7$  and  $\text{Sr}_4\text{Ti}_3\text{O}_{10}$  (space group  $I4/mmm$ ) [1–4]. The integer  $n$  can be related to the number of perovskite  $\text{SrTiO}_3$  layers interleaved with SrO rocksalt layers, as shown in figure 1. These  $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$  phases are functional materials due to superior dielectric properties as well as chemical and structural stability over a wide temperature range [1]. Furthermore, due to long-range lattice distortions induced by local deviations from the  $\text{SrTiO}_3$  stoichiometry caused by insertion of SrO layers, the  $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$  compounds are crystallographic shear phases according to Gutmann and co-workers [1]. Recently, it has been found that perovskite based crystals with the broken rotational symmetry may exhibit unexpected properties, such as superconductivity and large magnetoresistive anisotropy [5, 6].

It is interesting to note that these  $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$  compounds exhibit structural similarities to the so-called  $M_{n+1}AX_n$  phases (space group  $P6_3/mmc$ ), where M is a transition metal, A is mostly IIIA or IVA group element, X is either C or N and  $n = 1-3$  [7–9]. It has been argued that these phases constitute a new class of solids,

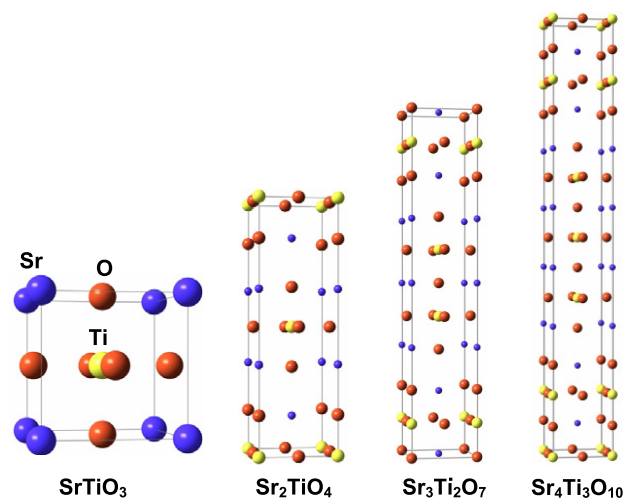


Figure 1. Structure of  $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$  phases.

where MX layers are interleaved with A layers [7]. Herein, these compounds are referred to as nanolaminates. In general,  $M_{n+1}AX_n$  phases are characterized by high elastic moduli [7, 8], they are machinable [10], they exhibit good damage tolerance [11], excellent thermal shock resistance [12], good corrosion resistance [13] and they are good thermal and electrical conductors [10]. It has also been observed that

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**Table 1.** Calculated lattice parameter ( $a$ ), tetragonal  $c/a$  ratio, bulk modulus ( $B$ ), elastic constant  $C_{44}$  and  $B/C_{44}$  ratio for  $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$  ( $n = \infty, 1-3$ ), SrO and TiO. Comparison is made with experimental data.

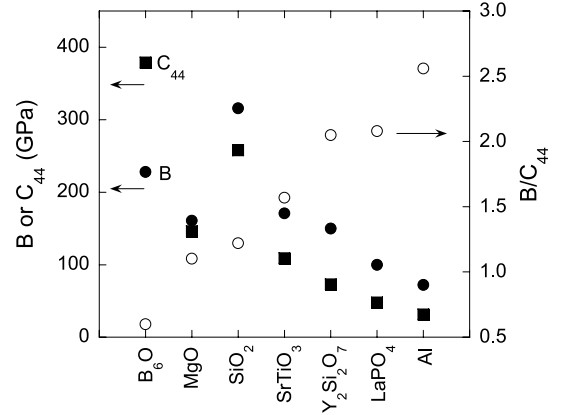
	$a$ (Å)	$c/a$	$B$ (GPa)	$C_{44}$ (GPa)	$B/C_{44}$
SrTiO <sub>3</sub> calc.	3.942	—	171	109	1.57
SrTiO <sub>3</sub> exp. [33]	3.901	—	174	124	1.41
Sr <sub>2</sub> TiO <sub>4</sub> calc.	3.899	3.285	137	95	1.44
Sr <sub>2</sub> TiO <sub>4</sub> exp. [3]	3.880	3.247	—	—	—
Sr <sub>3</sub> Ti <sub>2</sub> O <sub>7</sub> calc.	3.918	5.285	150	100	1.50
Sr <sub>3</sub> Ti <sub>2</sub> O <sub>7</sub> exp. [4]	3.900	5.226	—	—	—
Sr <sub>4</sub> Ti <sub>3</sub> O <sub>10</sub> calc.	3.918	7.314	156	103	1.51
Sr <sub>4</sub> Ti <sub>3</sub> O <sub>10</sub> exp. [4]	3.900	7.205	—	—	—
SrO calc.	5.199	—	86	64	1.34
TiO calc.	4.288	—	224	184	1.22

other phases crystallizing in the same space group (ternary phosphides [14],  $\text{Al}_3\text{BC}_3$  [15],  $\text{Zr}_2\text{Al}_3\text{C}_5$  [16] and  $\text{W}_2\text{B}_5$  based phases [17]) and the related space group  $P6/mmm$  ( $\text{Y}_{n+1}\text{Co}_{3n+5}\text{B}_{2n}$  [18]) as well as in the phases of the cubic  $Pm\bar{3}m$  symmetry (perovskite borides [19, 20] and nitrides [21, 22]) exhibit similar nanolaminated structures. Furthermore, similarities in the electronic structure and the elastic properties between these phases and  $\text{M}_{n+1}\text{AX}_n$  phases have been identified [8, 14–16, 18–22]. Hence, it can be argued that SrTiO<sub>3</sub> and SrO layers in  $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$  resemble MX and A layers in  $\text{M}_{n+1}\text{AX}_n$  phases. The elastic properties of  $\text{M}_{n+1}\text{AX}_n$  phases have been studied systematically [23–26], while the elastic properties of  $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$  are still unexplored.

In this work, we study the correlation between the electronic structure and elastic properties of  $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$  phases. These ternary oxides possess an unusually large bulk modulus to  $C_{44}$  ratio and the Peierls stress is comparably low. This may be understood based on the electronic structure: layers of low and high electron density are interleaved.

## 2. Theoretical methods

Calculations in this work were carried out using density functional theory [27], as implemented in the Vienna *ab initio* simulation program (VASP), wherein the projector augmented wave potentials with the generalized-gradient approximation are employed [28]. The following parameters were applied: convergence criterion for the total energy of 0.01 meV, Blöchl corrections for the total energy [29], cut-off of 500 eV, integration in the Brillouin zone according to Monkhorst–Pack [30] with  $7 \times 7 \times 7$  irreducible  $k$ -points and no spin polarization. Unit cells containing 5–34 atoms were relaxed with respect to atomic positions, internal free parameters and cell volumes. Bulk moduli were obtained by fitting the energy–volume curves using the Birch–Murnaghan equation of states [31]. Elastic constants have been obtained according to the method developed by Mehl and co-workers [32]. In order to study the chemical bonding, electron density distributions as well as total and partial density of states (DOS) were also calculated.

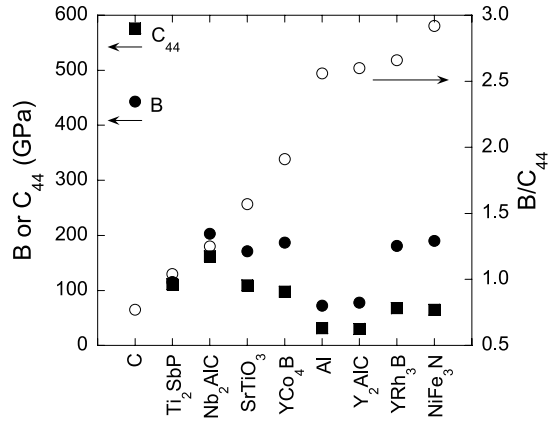
**Figure 2.** Bulk modulus ( $B$ ),  $C_{44}$  elastic constant and  $B/C_{44}$  ratio for a selection of oxides and Al.**Table 2.** Internal free parameters for  $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$  ( $n = \infty, 1-3$ ), as obtained by the VASP code. Comparison is made with experimental data.

	Ti 4e	Sr <sub>1</sub> 4e	Sr <sub>n</sub> 4e	O <sub>1</sub> 4e	O <sub>n</sub> 4e	O <sub>III</sub> 8g
SrTiO <sub>3</sub> calc.	—	—	—	—	—	—
Sr <sub>2</sub> TiO <sub>4</sub> calc.	—	0.354	—	0.159	—	—
Sr <sub>3</sub> Ti <sub>2</sub> O <sub>7</sub> calc.	0.098	0.315	—	0.194	—	0.096
Sr <sub>3</sub> Ti <sub>2</sub> O <sub>7</sub> exp. [4]	0.094	0.312	—	0.188	—	0.094
Sr <sub>4</sub> Ti <sub>3</sub> O <sub>10</sub> calc.	0.140	0.431	0.297	0.070	0.210	0.139
Sr <sub>4</sub> Ti <sub>3</sub> O <sub>10</sub> exp. [4]	0.136	0.432	0.296	0.068	0.204	0.136

## 3. Results and discussion

In table 1, the calculated values for lattice parameters, tetragonal  $c/a$  ratios, bulk moduli ( $B$ ) and elastic constants  $C_{44}$  for  $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$  phases are given. The calculated lattice parameters deviate by 0.5%–1.0% to the experimental values [3, 4, 33]. Internal free parameters, provided in table 2, deviate by 0.2%–4.1% to the experimental values [4].  $B$  and  $C_{44}$  values for Sr<sub>2</sub>TiO<sub>4</sub> ( $n = 1$ ) are 137 and 95 GPa, respectively, which accounts for the  $B/C_{44}$  ratio of 1.4. As  $n$  increases from 1 (Sr<sub>2</sub>TiO<sub>4</sub>) to  $\infty$  (SrTiO<sub>3</sub>),  $B$  and  $C_{44}$  increase to 171 and 109 GPa, respectively, and the  $B/C_{44}$  ratio increases to 1.6. The calculated  $B$  and  $C_{44}$  values for SrTiO<sub>3</sub> deviate by 0.2% and 13.8% to the experimental values, respectively [33]. The elastic properties of SrO and TiO (space group  $Fm\bar{3}m$ ) were also calculated for comparison and the values for the  $B/C_{44}$  ratio are 1.3 and 1.2, respectively. Clearly, the  $B/C_{44}$  ratio of the ternary is increased as compared to these binary oxides. This may have consequences for the deformability (or lack thereof) of these ternary oxides.

In order to analyse the here-obtained  $B/C_{44}$  ratios for the  $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$  phases, we provide a comparison with  $B/C_{44}$  ratios for a selection of oxides and nanolaminates, such as  $\text{M}_{n+1}\text{AX}_n$  phases. According to Pugh [34], the ratio of bulk and shear modulus represents a measure for ductile behaviour. Diamond and Al, for example, comprise a  $B/C_{44}$  ratio of 0.8 and 2.6, respectively [35]. It has been shown for  $\text{M}_{n+1}\text{AX}_n$  phases that Pugh’s notion for the brittle/ductile crossover is consistent with stress–strain relationship [36–39] as well as the Rice and the ZCT model [40–42]. In figure 2, the

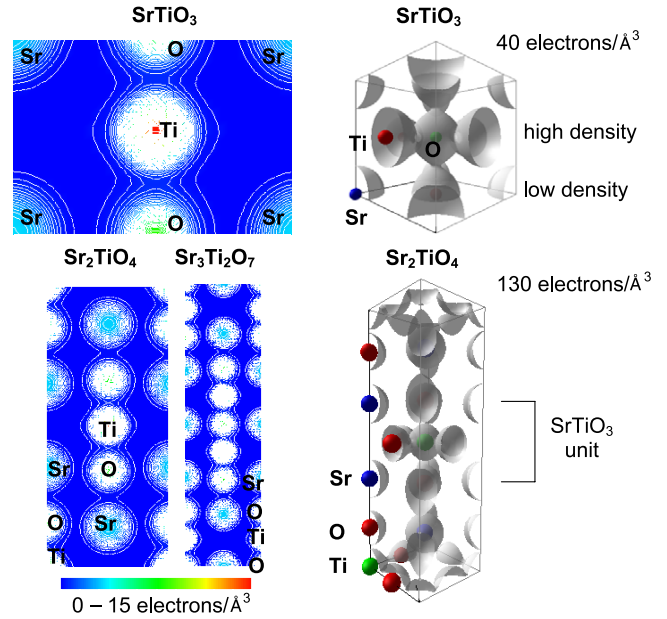


**Figure 3.** Bulk modulus ( $B$ ),  $C_{44}$  elastic constant and  $B/C_{44}$  ratio for a selection of nanolaminates as well as diamond and Al.

**Table 3.** Peierls stress ( $\sigma$ ) data for a selection of perovskites,  $M_{n+1}AX_n$  phases, and binary carbides.  $G$ ,  $\nu$ ,  $b$  and  $d$  designate the shear modulus, the Poisson's ratio, the Burgers vector and the interlayer distance between the glide planes, respectively.

	$G$ (GPa)	$\nu$	$b$ (Å)	$d$ (Å)	$\sigma$ (GPa)
SrTiO <sub>3</sub>	110	0.24	3.94	1.97	4.70
YRh <sub>3</sub> B	96 [19]	0.30 [19]	4.21	2.10	3.08
Ti <sub>2</sub> AlC	128 [25]	0.19 [25]	3.06	2.27	0.98
V <sub>2</sub> AlC	125 [25]	0.24 [25]	2.95	2.17	0.76
Cr <sub>2</sub> AlC	145 [25]	0.24 [25]	2.85	2.11	0.86
Nb <sub>2</sub> AlC	119 [25]	0.26 [25]	3.11	2.23	0.74
Ta <sub>2</sub> AlC	126 [25]	0.26 [25]	3.10	2.22	0.78
TiC	201 [49]	0.22 [49]	3.05	1.25	19.49
VC	236 [49]	0.23 [49]	2.92	1.18	22.87
CrC	200 [49]	0.25 [49]	2.84	1.16	17.46

elastic properties of SrTiO<sub>3</sub> are compared to Al (space group  $Fm\bar{3}m$  [35]), brittle oxides (B<sub>6</sub>O—space group  $R\bar{3}m$  [43], stishovite SiO<sub>2</sub>—space group  $P4_2/mnm$  [44], MgO—space group  $Fm\bar{3}m$  [45]) and oxides that were reported to be ductile, namely LaPO<sub>4</sub>—space group  $P2_1/n$  [46] and  $\gamma$ -Y<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>—space group  $P2_1/c$  [47]). The  $B/C_{44}$  ratio of SrTiO<sub>3</sub> is comparable to those reported for ductile oxides (LaPO<sub>4</sub>,  $\gamma$ -Y<sub>2</sub>Si<sub>2</sub>O<sub>7</sub>), but is by a factor of 1.3–2.6 larger than those of brittle oxides (B<sub>6</sub>O, stishovite SiO<sub>2</sub>, MgO). Based on the Pugh's notion [34] the here-presented  $B/C_{44}$  ratios of Sr <sub>$n+1$</sub> Ti <sub>$n$</sub> O <sub>$3n+1$</sub>  for  $n = 1, 2, 3, \infty$  suggest ductile behaviour. Hence, these ternary oxides may be prone to shearing and may be machinable. In figure 3, the elastic properties of SrTiO<sub>3</sub> are compared to a selection of nanolaminates (Nb<sub>2</sub>AlC and Y<sub>2</sub>AlC—space group  $P6_3/mmc$  [26, 36, 37], Ti<sub>2</sub>SbP—space group  $P6_3/mmc$  [14], YCo<sub>4</sub>B—space group  $P6/mmm$  [18], YRh<sub>3</sub>B—space group  $Pm\bar{3}m$  [20], NiFe<sub>3</sub>N—space group  $Pm\bar{3}m$  [21]) as well as diamond (space group  $Fd\bar{3}m$  [35]) and Al (space group  $Fm\bar{3}m$  [35]). Most of these phases exhibit a  $B/C_{44}$  ratio between diamond and Al, but YRh<sub>3</sub>B and NiFe<sub>3</sub>N even exceed the value for Al. Table 3 contains the estimated Peierls stress data for a selection of perovskites (SrTiO<sub>3</sub> and YRh<sub>3</sub>B),  $M_{n+1}AX_n$  phases (Ti<sub>2</sub>AlC, V<sub>2</sub>AlC, Cr<sub>2</sub>AlC, Nb<sub>2</sub>AlC and Ta<sub>2</sub>AlC) and rocksalt binary carbides (TiC, VC and CrC). The Peierls stress ( $\sigma$ ) can be used to estimate the initial stress



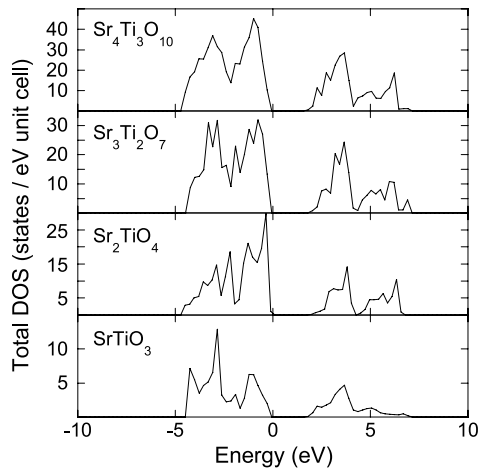
**Figure 4.** Electron density distribution for SrTiO<sub>3</sub>, Sr<sub>2</sub>TiO<sub>4</sub> and Sr<sub>3</sub>Ti<sub>2</sub>O<sub>7</sub> in the (110) plane. Electronic isosurfaces for SrTiO<sub>3</sub> and Sr<sub>2</sub>TiO<sub>4</sub> are also provided.

value required to initiate the movement of a dislocation in a glide plane [48]. The following expression was applied:

$$\sigma = \frac{2G}{1-\nu} \exp\left(-\frac{2\pi d}{b(1-\nu)}\right), \quad (1)$$

where  $G$  is the shear modulus,  $\nu$  is the Poisson ratio,  $b$  is the Burgers vector and  $d$  is the interlayer distance between the glide planes [48]. The  $G$  and  $\nu$  values for YRh<sub>3</sub>B,  $M_{n+1}AX_n$  phases and binary carbides were taken from literature [19, 25, 49]. The following Burgers vectors were considered: (001),  $1/3(1\bar{2}10)$  and  $1/2(110)$  for perovskites [50],  $M_{n+1}AX_n$  phases [38] and binary carbides [51], respectively. The  $d$  values were obtained for the following planes:  $1/2(001)$ ,  $(1/4 - z)(0001)$  and  $1/6(111)$  in perovskites,  $M_{n+1}AX_n$  phases and binary carbides [51], respectively, where  $z$  is the internal free parameter for M in  $M_{n+1}AX_n$ . The Peierls stress in these  $M_{n+1}AX_n$  phases is comparable to that in Al [48]. It is obvious that in the  $M_{n+1}AX_n$  phases dislocations can move, while this is not the case for the binary carbides. The here-studied perovskites exhibit an intermediate Peierls stress, approximately 4 times larger than in  $M_{n+1}AX_n$  phases, so that dislocation movement may be facilitated as well. Comparing the  $B/C_{44}$  ratios and Peierls stresses obtained for these nanolaminates, it can be speculated that the SrTiO<sub>3</sub> may also be prone to shearing and that all Sr <sub>$n+1$</sub> Ti <sub>$n$</sub> O <sub>$3n+1$</sub>  phases may have low Peierls stresses. In order to pinpoint the origin of this unusual behaviour, the chemical bonding is studied.

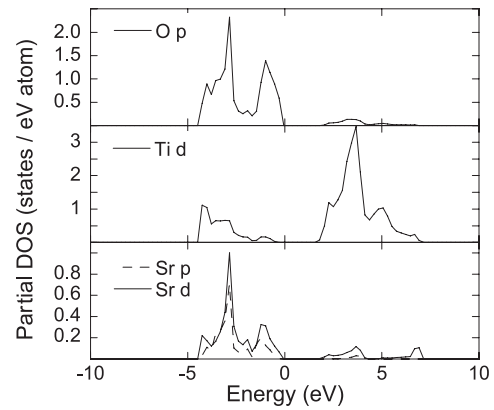
In figure 4, the electron density distributions for Sr <sub>$n+1$</sub> Ti <sub>$n$</sub> O <sub>$3n+1$</sub>  with  $n = 1, 2, \infty$  in the (110) plane are provided. For SrTiO<sub>3</sub>, it is evident that there are electrons shared between Ti and O, which is consistent with the notion of strong ionic-covalent interaction between these constituents.



**Figure 5.** Total DOS for SrTiO<sub>3</sub>, Sr<sub>2</sub>TiO<sub>4</sub>, Sr<sub>3</sub>Ti<sub>2</sub>O<sub>7</sub> and Sr<sub>4</sub>Ti<sub>3</sub>O<sub>10</sub>, as obtained by the VASP code. The Fermi level is set to 0 eV.

In perovskite oxides, it is commonly argued that ionic bonding dominates [33]. However, based on the Mulliken net charge analysis, covalent bonding between Ti and O in SrTiO<sub>3</sub> is also expected [33], as it can be seen in figure 4. While there is no charge shared between Ti–O (high electron density) and Sr (low electron density) layers, the whole (110) plane may be characterized by a uniform charge distribution of the Fermi gas. This is characteristic of metallic bonding. Also, there may be some ionic interaction between these constituents, but it may be screened by the Fermi gas. Figure 4 also contains the electronic isosurfaces for Sr<sub>n+1</sub>Ti<sub>n</sub>O<sub>3n+1</sub> with  $n = 1$  and  $\infty$  and hence the high/low electron density units are visible. For Sr<sub>2</sub>TiO<sub>4</sub> and Sr<sub>3</sub>Ti<sub>2</sub>O<sub>7</sub>, discrete SrTiO<sub>3</sub> units are bonded to weak Sr–O and further with metallic Ti–Sr and Ti–Ti units. Hence, the nature of chemical bonding is conserved as  $n$  in Sr<sub>n+1</sub>Ti<sub>n</sub>O<sub>3n+1</sub> changes, layers of high and low electron density are interleaved.

Figure 5 shows the total DOS for all compounds studied. There are several general remarks that can be made. All phases are insulators since there is a band gap in the order of 3 eV. This is consistent with previous work [33, 52]. The total DOS presented are similar. Therefore, we chose SrTiO<sub>3</sub> as a demonstrator compound and studied the chemical bonding in more detail. In figure 6, the partial DOS of SrTiO<sub>3</sub> is given. The chemical bonding is described with respect to lattice site as well as spin and orbital angular momentum quantum numbers. It is evident that the Ti and O states are hybridized and a weak interaction exists between Sr and O, which is consistent with previous work [33, 52]. This in turn indicates that the coupling between Ti–O and Sr layers in the (110) plane is weak, as shown in figure 4. In general, the coupling between ionic–covalent (Ti–O units with high electron density concentration) and metallic layers (Ti–Sr and Ti–Ti units with low electron density concentration) is weak. This is consistent with the notion that Sr<sub>n+1</sub>Ti<sub>n</sub>O<sub>3n+1</sub> compounds possess crystallographic shear planes [1]. We suggest that the  $B/C_{44}$  ratio is large due to this weak coupling, which in turn may enhance the ductility of these compounds. This is also consistent with the comparably low



**Figure 6.** Partial DOS for SrTiO<sub>3</sub>. The Fermi level is set to 0 eV.

Peierls stress, as discussed above. Based on the similarity in the elastic properties, estimated Peierls stresses and electron density distribution between the here-investigated compounds and the M<sub>n+1</sub>AX<sub>n</sub> phases as well as other nanolaminates, it is suggested that alternating covalent–ionic and metallic bonding in Sr<sub>n+1</sub>Ti<sub>n</sub>O<sub>3n+1</sub> phases may give rise to similar properties as observed for M<sub>n+1</sub>AX<sub>n</sub> phases.

#### 4. Conclusions

We have studied the correlation between the electronic structure and elastic properties of Sr<sub>n+1</sub>Ti<sub>n</sub>O<sub>3n+1</sub> ( $n = 1-3, \infty$ ). These ternary oxides possess a  $B/C_{44}$  ratio from 1.4 to 1.6, an unusually large ratio for oxides. The Peierls stress is comparably low, implying that dislocations may move in these compounds. This may be understood based on the electronic structure: ionic–covalent (Ti–O units possessing high electron density) are interleaved with metallic layers (Ti–Sr and Ti–Ti units possessing low electron density). We propose that the unusually large  $B/C_{44}$  ratio and low Peierls stress is a direct consequence of weak coupling between the ionic–covalent and metallic layers, causing a low  $C_{44}$  value, as well as strong coupling within ionic–covalent layers causing a large bulk modulus. Based on the similarity of the elastic properties, Peierls stresses and the electronic structure between the here-investigated ternary oxides and other nanolaminates including M<sub>n+1</sub>AX<sub>n</sub> phases, it is suggested that alternating covalent–ionic and metallic bonding may give rise to similar elastic properties as observed for M<sub>n+1</sub>AX<sub>n</sub> phases.

#### Acknowledgment

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