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To Construct Database for Norm-Conserving Pseudopotentials

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Pseudopotential database has been prepared as for H, Li, B, C, N, O, Na, Mg, Al, Si, P, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn and Sb. A partial core correction is considered to improve an overestimation of magnetic moments of transition metals (Fe, Co and Ni). As for prepared pseudopotentials, bulk properties (lattice constants, bulk moduli, electronic band structures etc.) are checked and they agree well with other theoretical and experimental results. There are no ghost bands in present electronic structure calculations using separable forms for non-local parts of pseudopotential.

1. Introduction

The first-principles molecular dynamics (FPMD) developed originally by Car and Parrinello[1] is a very powerful tool for performing an optimization of internal coordinates of atoms in a unit cell and electronic structures. Appearing this method, a dramatic reduction in storage and computing time is realized. Already, a variety of systems has been studied by many groups, and many remarkable achievements have been obtained.

A technique of total energy pseudopotential method is generally used in the FPMD. The basic concept of pseudopotential is a frozen core approximation which assumes that the electronic states of core electrons are insensitive to the neighboring atomic configuration. This assumption is valid in many cases of solid state physics. Therefore, avoiding core electrons and smoothing potentials, it is possible to use a plane wave basis set in the electronic structure calculation. In addition, it is relatively easy to formulate interatomic forces or stresses originated from Nielsen and Martin[2] in this approach.

Traditionally, empirical pseudopotentials [3] made in reproducing other (all-electron) theoretical or experimental results were used. However, such empirical pseudopotentials have a weak point that calculated pseudo charge densities do not agree with those of the real atoms even outside the core region.

In 1979, Hamann, Schlüter and Chiang[4] proposed a norm-conserving pseudopotential. This is constructed to reproduce eigen-values of valence states and norms of wave functions in all-electron calculations of atoms. A reliability of norm-conserving pseudopotentials is almost same level as other kinds of the first-principles all-electron calculation (LMTO, APW) in a variety of cases. Furthermore, Bachelet, Hamann and Schlüter[5] (BHS) reported a detailed description of making the norm-conserving pseudopotential and tabulated parameters of pseudopotentials fitted by analytic functions. Recently, Rappe, et al. and Troullier and Martin (TM)[6,7] proposed a new norm-conserving pseudopotential scheme to overcome a problem, in which a huge number of plane waves is required in the case of calculating first elements of atoms and transition metals. This is called 'optimized pseudopotential'.

Using pseudopotentials in the electronic structure calculation, one of the most serious problems is unphysical ghost bands which appear by using a separable form by Kleinman and Bylander[8] in order to reduce a cost of the numerical calculation. There is no way to overcome easily such a problem without any try and error. Although some technical treatments avoiding ghost bands are given in reports[9,10], it requires a knowledge of the first-principles calculation and a way of making pseudopotentials. The author thinks that it is efficient and useful to prepare a database of norm-conserving pseudopotentials as the other way of approach to solve the above problem. Already, pseudopotentials for over 30 kinds of atoms have been prepared.

In this proceeding, it is described the outline of pseudopotential database and calculational method of the electronic structure calculation in section II. In section III, results of

accuracy for the database (bulk properties, electronic band structures for transition and noble metals) are presented. Section IV is devoted to summary of this study.

2. Method of Calculation

2.1 Outline of pseudopotential database

At present, norm-conserving pseudopotentials for H, Li, B, C, N, O, Na, Mg, Al, Si, P, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn and Sb are available. Pseudopotentials for Ca, Ga, Ge, Rb and Sr are preparing and testing. Li, Na, Mg, Al, Si and P are constructed by using the way of BHS[5], the other is for the optimized pseudopotentials by TM[7]. In this database, it is checked that there are no ghost bands as a result of the electronic structure calculation for solid even by using separable forms[8]. As for transition and noble metals, non-local parts of s, p and d pseudopotentials are used. In this case, a core potential $V_{\text{core}}(\mathbf{r})$ is used as a local pseudopotential based on BHS[5]. Parameters of $V_{\text{core}}(\mathbf{r})$ are appropriately adjusted to avoid ghost bands in this work. As for the other pseudopotentials(H, Li, Na, B, C, N, O, Mg, Al, Si, P, In, Sn and Sb), non-local parts are s and p in which the d part of pseudopotential is treated as a local one. Pseudopotentials for empty states (for examples $4p$ states of $3d$ transition metals) are made in a condition of ionic configuration for valence electrons in the same way of BHS[5]. A scalar relativistic effect is considered to these pseudopotentials[11]. This effect is important in the case of $4d$ transition metals.

The name of this database is 'NCPS95'(Norm-Conserving Pseudopotential 1995). Calculated results of bulk properties for transition and noble metals and alloys will be presented in the next section in detail. With regards to the results of other atoms, another papers of the author and colleagues are available for references[12,13,14,15].

2.2 Electronic band structure calculation

The present electronic structure calculation is based on the local (spin) density approximation(L[S]DA)[16,17] in the density functional theory[18,19]. In this study, two types of local (spin) density approximation for exchange-correlation are used. The electronic part is optimized by using the steepest descent type of algorithm which is modified to accelerate a convergence of the total energy[20].

Although the optimization of only the electronic part is performed in this work, if necessary, it is possible to optimize interatomic coordinates in a unit cell and unit cell shapes using forces acting on atoms and stresses [2] on unit cell surfaces, respectively, in this computer code.

3. Results and Discussion

3.1 Bulk properties and electronic band structures of transition and noble metals

Calculated bulk properties and electronic band structures will be presented as for Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag and Cd. The bulk properties (equilibrium lattice constants and bulk moduli) are tabulated in Table I. In this table, results of second column are present work, third is the all-electron band structure calculation[21] and fourth is the experimental data of Kittel[22]. Left values of every column are equilibrium lattice constants(\AA), and right ones are bulk moduli(Mbar). Almost results are calculated in a bcc or fcc structure(see Table I). As for only Zn and Cd, bulk properties and electronic band structures are calculated in a hcp structure, in which c/a ratios of Kittel[22] are employed. Although the hcp structure is more stable than the fcc structure in many cases, the fcc structure is adopted in order to compare the reference data of calculation[21]. In addition, it is difficult to optimize c/a ratios of every hcp structure because of computer resources, although it is possible to optimize the unit cell shape (c/a ratio) by using stresses.

In this table, the bulk properties agree with other theoretical and experimental data within 2~3 % for equilibrium lattice constants and 10~20 % for bulk moduli without a few exceptions. In the cases of Ti, V, Fe and Pd, disagreement is more than 2% for equilibrium lattice constants. Particularly, the lattice constant of Fe(paramagnetic) in this work is 3.9 % shorter than that of experiment. Since the values of bulk moduli depend tightly on a way of fitting and calculational condition(energy cutoff, a number of sampling k points, etc), the difference of about 15 ~ 20 % is not so serious.

Conditions of calculation for every case are also shown in table I. The energy cutoff is usually 81Ry. In a few cases, it is 144Ry(see Table I). A number of sampling k points are 55 (bcc), 89 (fcc) and 95(hcp) in an irreducible first Brillouin zone(BZ). The Wigner interpolation formula for exchange-correlation[16] in a paramagnetic phase is used.

There are no ghost bands as a result of checking calculated electronic band structures. Logarithmic derivatives for pseudo and real atomic wave functions in all most cases are also checked. Agreements of each other are well in almost cases. About a few cases, although there is no problem in electronic band structures, it is necessary to investigate a further analysis of calculated results and logarithmic derivatives in future study.

In the next stage, ferromagnetic phases of Fe, Co and Ni are calculated. Recently, some papers[23,24] suggest that it is necessary to consider a partial core correction (PCC)[25] in order to improve overestimated values of magnetic moments. With the PCC (Fe, Co and Ni), calculated results of equilibrium lattice constants, bulk moduli and magnetic moments are tabulated in Table II. The calculated magnetic moment of Ni without PCC is $0.8\mu_B$ which is overestimated on the comparison of the other calculated value[21] ($0.59\mu_B$), and improved with PCC ($0.603\mu_B$). In the paramagnetic phase of Fe, the calculated value of the equilibrium lattice constant is underestimated in the difference order of 3.9% on

the comparison of the experimental value. On the other hand, the difference order of the equilibrium lattice constant is improved to 2.3% in the ferromagnetic case. Electronic band structures for Fe, Co and Ni(ferromagnetic) are shown in Fig. 1 (a),(b) and (c), respectively. The overall trend of the dispersion curves for above band structures agrees well with the other theoretical results[21,24].

Calculational conditions are as follows: values of energy cutoff and a number of sampling k points in an irreducible BZ are 81Ry (for Fe, Co, Ni), 121Ry(for Ni), 55 (for Fe[bcc]) and 89(for Co,Ni[fcc]), respectively. The LSDA formula by Moruzzi, Janak and Williams[17] is used for Fe, Co and Ni.

It is possible to calculate stresses[2] acting on unit cell surfaces in this code of program. This lead to an automatic optimization of a unit cell shape under a constant pressure condition. The difference order of the equilibrium lattice constants from total energies and stresses is about 0.6% in the case of 81Ry. Calculated values of stresses and total energies as a function of volume are shown in Fig. 2 for Ni(121Ry, ferromagnetic). It is found that the agreement with the minimum of total energy and the zero point of stress is improved within 0.3% for the lattice constant (1.0% for volume). This difference (0.3%) would be improved in a condition of increasing energy cutoff.

It is necessary to consider a correction term of PCC in the stress calculation. A detailed formulation of this correction will be presented in Appendix.

3.2 Calculation for alloys (*NbMo, CoAl and NiAl*)

Alloys of NbMo, CoAl and NiAl are calculated as a CsCl type crystal structure in order to check accuracy of pseudopotentials (related to transferability). Calculational conditions are as follows. An energy cutoff is 81Ry, a number of sampling k-points is 84 in an irreducible BZ. Calculated bulk properties (NbMo, CoAl and NiAl) and electronic band structure (CoAl) are shown in Table I and Fig. 3, respectively. In all cases, they are treated as paramagnetic. Equilibrium lattice constants agree quite well with other theoretical and experimental results[26,27]. The agreement of the overall trend of dispersion curves between this work and that by the electronic band structure calculation for CoAl[26] is quite well.

4. Summary

Database of norm-conserving pseudopotentials for over 30 kinds of atoms has been constructed. The bulk properties and electronic band structures of them are calculated and checked accuracy. Calculated results given no ghost bands agree well with other theoretical and experimental results without a few exceptions.

The purpose of this database is as follows. It is possible to perform the optimization of electronic, interatomic and unit cell shape structures in a system of an arbitrary combination of atoms in a variety of environments (complex compounds, surfaces, interfaces,

impurities[defects] and clusters, etc.), using this database with the first-principles electronic structure calculation. This procedure will lead to prediction (or creating) of new materials, or support to synthesize new materials in experiment. Also, it will be possible to search a new chemical reaction process and solid state characteristics. Therefore, the final purpose of this study is to design new materials by using this database in the FPMD. The author expects that using this database is the first step of this purpose.

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Appendix: Derivation of the correction term of stress for PCC

Here, the derivation of the correction term of stress for PCC is described in detail. The following equation is the starting point in a non-spin polarized case.

$$\frac{\partial(\Omega\epsilon_{xc}(\mathbf{G})\rho(\mathbf{G}))}{\partial\epsilon} = \Omega\rho_c\epsilon_{xc}(\mathbf{G}) + \Omega\frac{\partial\rho_c(\mathbf{G})}{\partial\epsilon}\epsilon_{xc}(\mathbf{G}) + \Omega\rho(\mathbf{G})\frac{\partial\epsilon_{xc}(\mathbf{G})}{\partial\epsilon}, \quad (1.1)$$

where ϵ_{xc} is an exchange-correlation energy, ρ a total charge density, ρ_c a charge density of partial core, Ω a volume, ϵ a distortion and \mathbf{G} reciprocal lattice vectors. In this equation, $\Omega\rho_v$ is invariant in the lattice distortion ϵ , in which ρ_v is a charge density of valence electrons $\rho = \rho_v + \rho_c$.

The third term at the right hand side of equation (1) is derived as follows.

$$\frac{\partial\epsilon_{xc}(\mathbf{G})}{\partial\epsilon} = \frac{1}{\Omega} \int \frac{\partial\epsilon_{xc}(\mathbf{r})}{\partial\epsilon} e^{-i\mathbf{G}\mathbf{r}} d\mathbf{r}, \quad (1.2)$$

$$\frac{\partial\epsilon_{xc}(\mathbf{r})}{\partial\epsilon} = \frac{1}{\Omega} \int \left(\frac{\partial\rho_v}{\partial\epsilon} + \frac{\partial\rho_c}{\partial\epsilon} \right) \frac{\mu_{xc} - \epsilon_{xc}}{\rho_v + \rho_c} e^{-i\mathbf{G}\mathbf{r}} d\mathbf{r}, \quad (1.3)$$

$$= \frac{1}{\Omega} \int \frac{\rho_v}{\rho_v + \rho_c} (\epsilon_{xc} - \mu_{xc}) e^{-i\mathbf{G}\mathbf{r}} d\mathbf{r} + \frac{1}{\Omega} \int \frac{\partial\rho_c(r)}{\partial\epsilon} \frac{\mu_{xc} - \epsilon_{xc}}{\rho_v + \rho_c} e^{-i\mathbf{G}\mathbf{r}} d\mathbf{r}. \quad (1.4)$$

$$\frac{\partial\rho_c(r)}{\partial\epsilon} = \sum_{\mathbf{G}} \left\{ \frac{\partial}{\partial\epsilon} \left(\frac{1}{\Omega} \int \rho_c(r) e^{-i\mathbf{G}\mathbf{r}} d\mathbf{r} \right) e^{i\mathbf{G}\mathbf{r}} \right\} \quad (1.5)$$

$$= - \sum_{\mathbf{G}} \rho_c(\mathbf{G}) e^{i\mathbf{G}r} + \sum_{\mathbf{G}} \left\{ \frac{1}{\Omega} (-2G_\alpha G_\beta) \left(-\frac{1}{2G} \right) \int \rho_c(r) (j_1(Gr)) r^3 dr \right\} e^{i\mathbf{G}r}, \quad (1.6)$$

where μ_{xc} is an exchange-correlation potential.

Therefore,

$$\begin{aligned} \frac{\partial \epsilon_{xc}(\mathbf{G})}{\partial \epsilon} &= \frac{1}{\Omega} \int (\epsilon_{xc}(\rho(r)) - \mu_{xc}(\rho(r))) e^{-i\mathbf{G}r} d\mathbf{r} \\ &+ \frac{1}{\Omega} \int \left(\sum_{\mathbf{G}} P_c(\mathbf{G}) e^{i\mathbf{G}r} \right) \frac{\mu_{xc} - \epsilon_{xc}}{\rho_v + \rho_c} e^{-i\mathbf{G}r} d\mathbf{r}, \end{aligned} \quad (1.7)$$

where

$$P_c(\mathbf{G}) = -2G_\alpha G_\beta \left(\frac{1}{2G} \right) \int \rho_c(r) (j_1(Gr)) r^3 dr. \quad (1.8)$$

The final formula is

$$\begin{aligned} \frac{\partial}{\partial \epsilon} (\Omega \epsilon_{xc}(\mathbf{G}) \rho(\mathbf{G})) &= \Omega (\epsilon_{xc}(\mathbf{G}) - \mu_{xc}(\mathbf{G})) (\rho_v(\mathbf{G}) + \rho_c(\mathbf{G})) + \Omega P_c(\mathbf{G}) (\mu_{xc}(\mathbf{G}) - \epsilon_{xc}(\mathbf{G})) \\ &+ \Omega \epsilon_{xc}(\mathbf{G}) \frac{\partial \rho_c(\mathbf{G})}{\partial \epsilon}. \end{aligned} \quad (1.9)$$

It is possible to expand this formula in a spin polarized case. The charge density ρ is divided ρ_\uparrow and ρ_\downarrow , and also the exchange-correlation potential μ_{xc}^\uparrow and μ_{xc}^\downarrow .

In the first term of right hand side at above equation, μ_{xc} is divided as $\frac{1}{2}(\mu_{xc}^\uparrow + \mu_{xc}^\downarrow)$.

The second term is reformulated as the same way,

$$(\text{The second term}) = \Omega P_c(\mathbf{G}) \left(\frac{\mu_{xc}^\uparrow(\mathbf{G})}{2} + \frac{\mu_{xc}^\downarrow(\mathbf{G})}{2} - \epsilon_{xc}(\mathbf{G}) \right). \quad (1.10)$$

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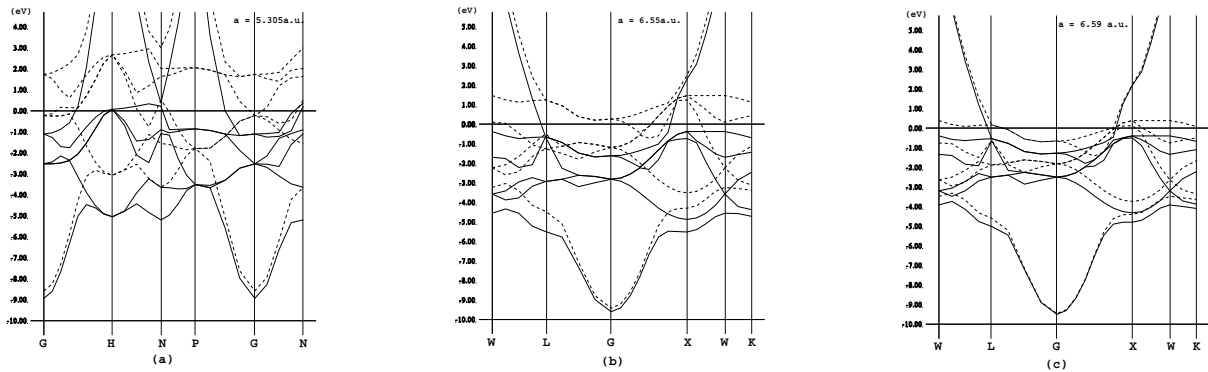


Fig.1. Calculated electronic band structures for Fe, Co and Ni in ferromagnetic are plotted at (a), (b) and (c), respectively. The Fermi level is indicated by horizontal line. Values of lattice constants are indicated in every figure. Dashed curves are for minority spin and solid curves for majority spin.

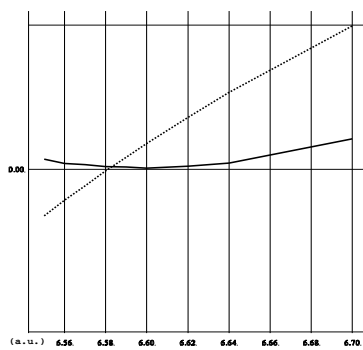


Fig. 2. The total energy and stress of Ni(121Ry, ferromagnetic) as a function of lattice constants are plotted. Solid curve is for the total energy, and dashed curve for the stress.

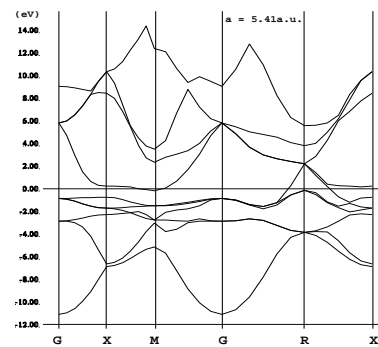


Fig. 3. The dispersion curve for CoAl alloy. The Fermi level is indicated by horizontal line. The lattice constant is 5.41a.u.

Table 1. Calculated bulk properties (equilibrium lattice constants and bulk moduli) and calculational conditions (energy cutoff and crystal structure) for transition and noble metals are tabulated. Unit of lattice constant is Å , bulk modulus Mbar and energy cutoff Ry, respectively. Left values are for lattice constants and right values for bulk moduli in every column. Numerical values at parentheses denoted in a unit of % means the difference of order for present values from other theoretical or experimental results. The values of block for hcp Zn and Cd are lattice constants of a and c, respectively, bulk moduli are not calculated. 'ASW' denotes the all-electron calculation (ASW), see reference[28].

	present work		MJW		Exp	
Ti(bcc)	3.254	1.183			3.327	(2.2%)
Ti(bcc)	3.228	1.152	(pcc)		3.327	(3.0%)
Ti(fcc)	4.064		4.00	(1.6%)	1.16	
V(bcc)	2.999	1.833	2.932	(2.3%)	1.64	3.03 (1.0%) 1.619
Cr(bcc)	2.81	2.931	2.805	(0.2%)	2.70	2.88 (2.4%) 1.901
Cu(fcc 81Ry)	3.622	1.62	3.577	(1.3%)	1.55	3.61 (0.3%) 1.37
Cu(fcc 144Ry)	3.64	1.43	3.577	(1.8%)	1.55	3.61 (0.8%) 1.37
Zr(fcc)	4.448	0.954	4.403	(1.0%)	0.94	
Nb(bcc)	3.266	1.81	3.281	(0.5%)	1.68	3.3 (0.1%) 1.702
Mo(bcc)	3.144	2.78	3.117	(0.9%)	2.51	3.15 (0.2%) 2.725
Zn(fcc)	3.921	0.76	3.837	(2.2%)	0.82	
Zn(hcp)	(2.66,4.95)				(within 1%)	
Cd(fcc 81Ry)	4.519	0.506	4.445	(1.7%)	0.461	
Cd(fcc 144Ry)	4.507		4.445	(1.4%)	0.461	
Cd(hcp 81Ry)	(3.032,5.718)				(within 1.75%)	
Pd(fcc)	3.99	1.7	3.93	(1.6%)	1.7	3.89 (2.6%) 1.808
Ag(fcc)	4.157	1.04	4.122	(0.8%)	1.02	4.09 (1.6%) 1.007
Sc(fcc)	4.499	0.52	4.493	(0.1%)	0.57	
Y(fcc)	4.896	0.44	4.884	(0.2%)	0.33	
Y(fcc)	4.880	0.46	4.884	(0.1%)	0.33	($E_f - 7$ eV ghost)
Tc(fcc)	3.884	3.26	3.852	(0.8%)	2.93	
Fe(bcc)	2.759	3.14	2.725	(1.2%)	3.06	2.87 (3.9%) 1.68
Co(fcc)	3.453	2.61	3.412	(1.2%)	2.84	
Ni(fcc)	3.511	2.28	3.466	(1.3%)	2.20	3.519 (0.2%) 1.86
Ru(fcc)	3.833	3.38	3.810	(0.6%)	2.89	
Rh(fcc)	3.867	2.93	3.831	(0.9%)	2.61	3.800 (1.8%) 2.70
NbMo(CsCl)	3.195	2.52			3.203	(0.2%)
CoAl(CsCl)	2.808	1.89	2.805	(0.1%)	(1.99)	2.861 (1.6%) 1.62
NiAl(CsCl)	2.854	1.64	2.868	(0.5%)	(ASW)	

Table 2. Calculated bulk properties (equilibrium lattice constants[left], bulk moduli[middle] and magnetic moments[μ_B ,right]) for ferromagnetic Fe, Co and Ni are tabulated. In the case of Ni(81Ry), the equilibrium lattice constant and bulk modulus are not calculated. The magnetic moment (Ni,81Ry) is obtained at 3.466 Å. 'pcc' indicates considering the partial core correction. The form of table is the same of Table 1, exception for appending values of magnetic moments. In the column of experimental results, lattice constants (left) and bulk moduli (right) are only presented.

	present work			MJW				Exp	
Fe(bcc,pcc)	2.805	2.18	2.25	2.789	(0.6%)	2.17	2.15	2.87	(2.3%) 1.683
Co(fcc,pcc)	3.484	2.64	1.61	3.461	(0.7%)	2.40	1.56		
Ni(fcc,81Ry)	-	-	0.8						
Ni(fcc,81Ry,pcc)	3.487	2.35	0.602	3.466	(0.6%)	2.27	0.59	3.52	(0.9%) 1.86
Ni(fcc,121Ry,pcc)	3.485	2.37	0.603	3.466	(0.6%)	2.27	0.59	3.52	(1.0%) 1.86