

# A New Type of the Interatomic Potential

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(Received September 30, 1986)

## Abstract

The homo-nuclear interatomic potentials between Dirac-Hartree-Fock-Slater atoms are calculated within the frame work of the statistical model including exchange correlation interaction. Of these, Xe-Xe potential can reproduce reasonably the experimental data of the differential scattering cross section. We find that a simple screening function expresses these precise potentials analytically. A Table of the parameters of screening functions is given for the diatomic systems of atoms from  $Z=2$  to  $Z=92$ . A screening function to represent those potentials is as well proposed for practical use.

## 1. Introduction

The analysis of the phenomena concerning with low energy atomic collisions can be estimated by the interatomic potential (IP) through the classical orbital equation. The low energy atomic collisions, especially in the LSS reduced energy unit  $\epsilon < 1$ , are considered to lose the incident energy of projectiles by nuclear stopping processes mainly. And the shell effects attributed to the atomic structures have been observed in this energy range [1, 2, 3]. Then the precise IP is needed to describe atomic collisions reasonably in that energy region. There have been two kinds of streams of the investigations for IP: One approach intends to have the general description of atomic collisions in reduced units for the sake of practical use. Another intends to have the precise potential in order to explain the atomic number dependence or the shell effect observed experimentally.

As for the former intention, Firsov derived generally the universal function

expressing the IP and a reduced length of the diatomic system based on the Thomas-Fermi statistical model and variational method [4]. Lindhard established the general theory to describe the atomic collisions, which was called as LSS theory [5]. On the other hand, as for the latter intention the basic formalism written by charge density functional [4] had been improved by adding the contribution of the higher order term, i.e., the exchange term [6, 7, 8] and the exchange correlation term [9]. Furthermore, the realistic charge densities of the atoms have been used, e.g., Thomas-Fermi-Dirac (TFD) [6, 7], Hartree-Fock (HF) [8], Hartree-Fock-Slater (HFS) [10, 11], and Dirac-Hartree-Fock-Slater (DHFS) [1, 12]. There seems, however, no sufficient agreement between calculations and experiments of differential cross section [1, 12] to exist.

In our previous work, some of IPs were calculated according to the Gordon-Kim statistical model [9] using DHFS charge density of atoms [13]. We had pointed out that the oscillation exists in screening functions, which were evaluated as the exponents of the power potentials at certain low energy region. Similar oscillation was reported in other calculations [14, 15], too. In fact these exponents are very important to explain the oscillatory target dependence of the measured sputtering yield [16].

In the present work, the IPs have been calculated for the systems of atoms from  $Z=2$  to  $Z=92$  in the same manner to the previous work. The potentials have shown not only the oscillation qualitatively but also being precise quantitatively, because it can reproduce the differential scattering cross section of measured data reasonably.

Then those potentials have been expressed analytically in a simple screening function for further applications. The screening function is usually written as a function of a reduced length, however, the present results recommend not to scale IPs by a single screening length. This problem of scaling has been discussed by Biersack et al. theoretically [11] and other authors empirically [17, 18].

The purpose of the present work is to show that our calculation of IPs is satisfactory and to express each homo-nuclear IP in analytical screening function. The screening function suggested here has only three parameters and is very simple for applications.

2. The interatomic potential

The homo-nuclear IPs are calculated according to the Gordon-Kim statistical model. The formalism to calculate them is expressed by the sum of four terms;  $V_{el}$  electrostatic term,  $V_k$  kinetic term,  $V_{ex}$  exchange term, and  $V_{cor}$  correlation term as follows;

$$V(R) = V_{el} + V_k + V_{ex} + V_{cor} \tag{1}$$

$$V_{el} = \frac{1}{2} \left[ \frac{Z_1 Z_2^*(R)}{R} + \frac{Z_2 Z_1^*(R)}{R} \right] - \frac{1}{2} \left[ \int_{|\vec{r}|=0}^{\infty} \frac{Z_1^*(r) \rho_2(\vec{r}-\vec{R})}{|\vec{r}|} d\vec{r} + \int_{|\vec{r}-\vec{R}|=0}^{\infty} \frac{Z_2^*(r) \rho_1(\vec{r})}{|\vec{r}-\vec{R}|} d\vec{r} \right], \tag{2}$$

$$V_k = \frac{3}{10} (3\pi^2)^{2/3} \int_{|\vec{r}|=0}^{\infty} \left[ \rho_{12}(\vec{r})^{5/3} - \rho_1(\vec{r})^{5/3} - \rho_2(\vec{r}-\vec{R})^{5/3} \right] d\vec{r}, \tag{3}$$

$$V_{ex} = -\frac{3}{4} \left[ \frac{3}{\pi} \right]^{1/3} \int_{|\vec{r}|=0}^{\infty} \left[ \rho_{12}(\vec{r})^{4/3} - \rho_1(\vec{r})^{4/3} - \rho_2(\vec{r}-\vec{R})^{4/3} \right] d\vec{r}, \tag{4}$$

$$V_{cor} = \int_{|\vec{r}|=0}^{\infty} \epsilon_{cor}(\vec{r}) \rho_{12}(\vec{r}) d\vec{r}, \tag{5}$$

$$Z^*(r) = Z - \int_{|\vec{r}'|=0}^{\infty} \frac{\rho(\vec{r}')}{|\vec{r}-\vec{r}'|} d\vec{r}' \tag{6}$$

where  $Z^*(r)$  is the equivalent positive charge of the atom at the distance  $r$  from either nucleus,  $R$  the internuclear distance,  $\epsilon_{cor}$  the correlation interaction [9], and  $\rho(r)$  of DHFS atom [13]. The shell effect in  $Z^*(r)$  of DHFS atom is shown in Fig. 1 in the case of Xe atom. The charge density of the diatomic system is assumed to be expressed by the superposition of the charge density of two

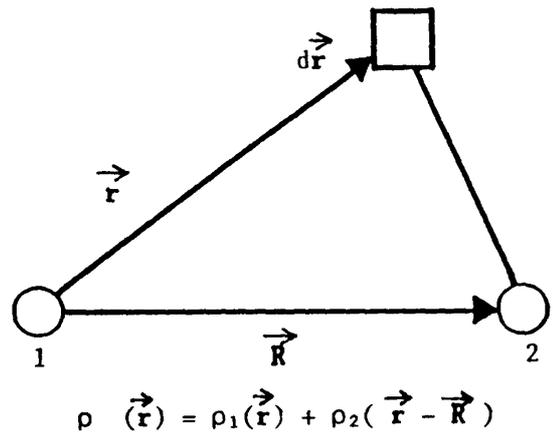
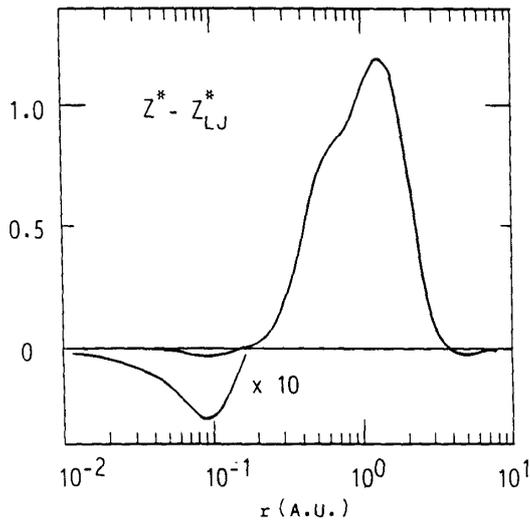


Fig. 1 Shell effect of Xe atom are illustrated as  $Z^*-Z^*_{LJ}$ .  $Z^*$  are of DHFS atom, and  $Z^*_{LJ}$  are of LJ (Lenz-Jensen potential [19]) atom.

Fig. 2 Geometry used in calculating the interaction energy between two atoms separated by  $R$ . The number 1 and 2 denote the locations of the nuclei.  $d\vec{r}$  is an arbitrarily chosen volume element containing electrons of both atoms.

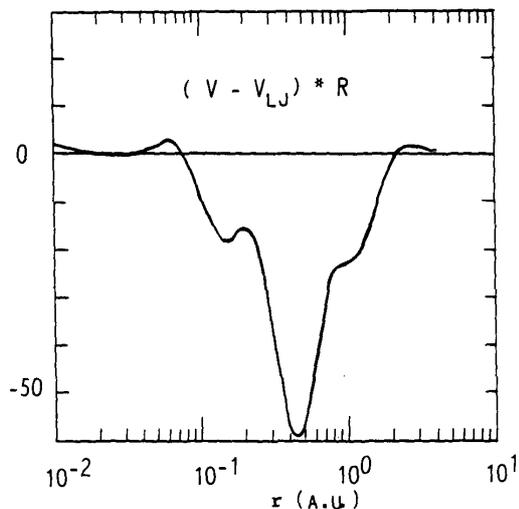


Fig. 3 The potential difference between potential of DHFS atoms and that of LJ atoms is illustrated. The atoms are Xe.

isolated atoms as illustrated in Fig. 2. Here all of homo-nuclear IPs from  $Z=2$  to  $Z=92$  are calculated according to Eq. (1). The shell effect appears also in the IP as is shown in Fig. 3. It seems strange that the quantities illustrated in Fig. 1 and 3 show the opposite sign, however, the electrostatic contribution is negative in this range of the internuclear distance [9].

### 3. Accuracy of the potential calculation

The first purpose of this work is to estimate the accuracy of our potential calculation. We had already suggested qualitatively that IPs show  $Z$  oscillation or shell effect of atoms [16]. The oscillation in the exponents of the power potential at certain low energy region supports the  $Z$  oscillation of the sputtering yield. On the other hand, there are some experiments to indicate the shell-shell matching in the atomic collisions even in the low energy region [1, 2, 3]. In this work we calculate the differential scattering cross section using our calculated potential and orbital equation, in order to check the accuracy of our potential quantitatively. The result is compared with experiment [1] for the case of Xe-Xe collision of 100 Kev as is shown in Fig. 4. The present calculation for the potential is known to be quantitatively reasonable.

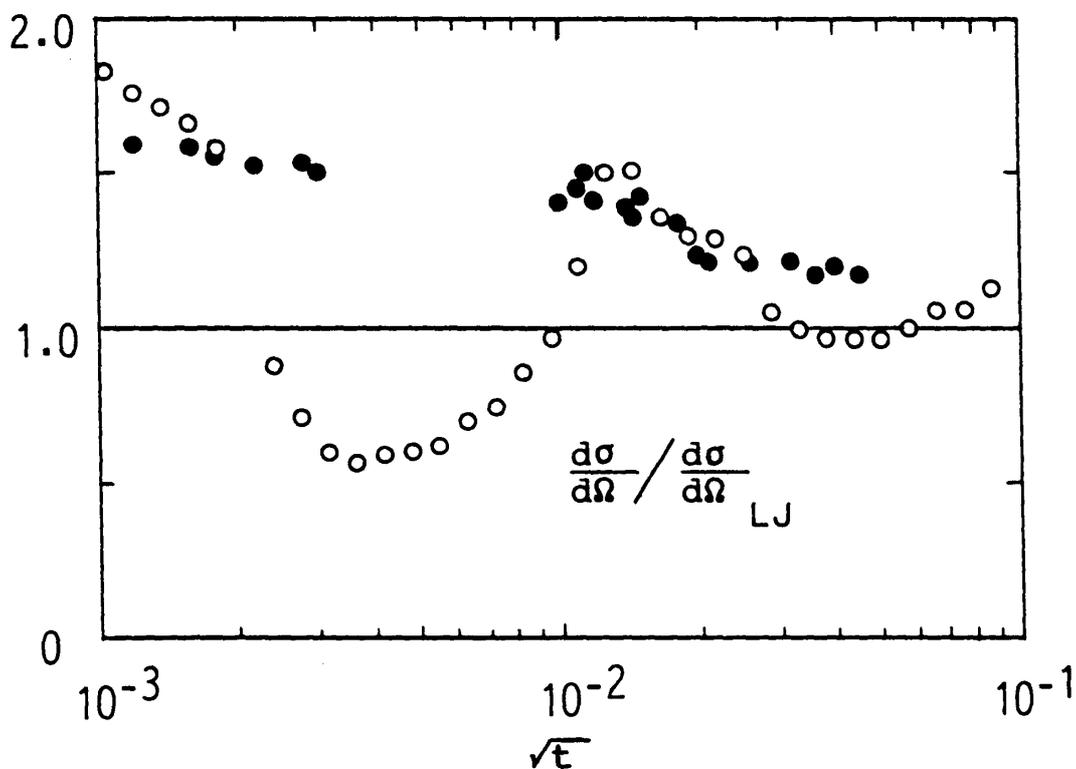


Fig. 4 The ratio of the differential scattering cross section due to the present potential to that due to universal LJ potential. The present results are denoted by open circles with comparison to the measured data denoted by solid circles. The experimental data are by Loftager et al. [1] in the case of Xe-Xe of 100 kev. The abscissa is the transfer energy  $\sqrt{\epsilon} = \epsilon \sin^2(\theta/2)$ , where  $\theta$  is the scattering angle in the c.m. system,  $\epsilon$  LSS reduced energy.

#### 4. Screening function

The second purpose of this work is to express the precise homo-nuclear IPs into some analytical screening function for convenience. The properties of the screening function itself and its parameters will help us to understand the IPs more clearly and systematically. We find that the following function can be one of the best screening functions  $\psi(R/a) = V(R) R/Z^2$  for all IPs calculated here;

$$\psi(x) = \exp(-Ax + Bx^{1.5} - Cx^2) \quad (7)$$

where  $x = R/a$  is the reduced length,  $a$  the screening length. This type of potential is called as MLJ (modified Lenz-Jensen) potential hereafter since it coincides to Lenz-Jensen potential for small  $x$ . The fitness of MLJ potential

to the calculated IPs is shown in Fig. 5. MLJ potential is known to follow well the numerical IPs. The problem that this function is appropriate or not as the screening function is reviewed in Appendix.

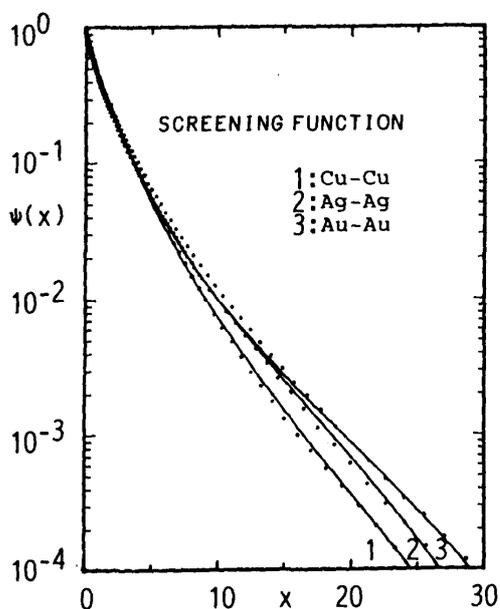


Fig. 5

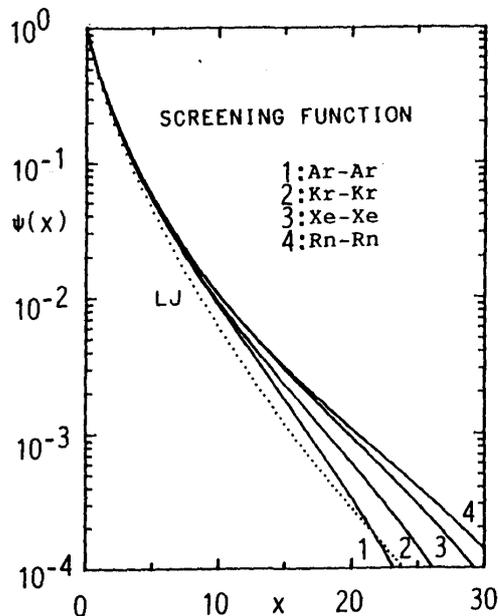


Fig. 6

Fig. 5 The fitness of MLJ potential to the calculated homo-nuclear IPs according to Eq. (1). Solid lines are MLJ potentials and associated marks are the corresponding numerically calculated ones. The abscissa is the reduced length  $x = R/a$ , where  $a$  is the Lindhard screening length.

Fig. 6 The  $Z$  dependence of homo-nuclear screening functions, where the Lindhard screening length is used. All of these atoms are noble elements in 8th row of the Periodic Table.

The three parameters  $A$ ,  $B$ , and  $C$  have been determined by the least square analysis. In Fig. 6 MLJ potentials for atoms of noble elements (8th row) are plotted. This Figure tells us that the Lindhard screening length is not appropriate to bunch the IPs into a single screening function in this case. Dotted line denotes Lenz-Jensen potential. In fact three kinds of parameters  $A$ ,  $B$ , and  $C$  for respective IPs for atoms of  $Z = 2$  to  $Z = 92$  show the different  $Z$  dependences to each other. Roughly speaking, all of three parameters seem to decrease with increasing atomic number  $Z$ . This fact supports that the used screening length is not appropriate in a strict meaning. This tendency is expressed in the next relations;

$$\begin{aligned}
 \bar{A} &= 1.20 & Z^{-0.0436} \\
 \bar{B} &= 0.368 & Z^{-0.111} \\
 \bar{C} &= 0.0566 & Z^{-0.258}
 \end{aligned}
 \tag{8}$$

This result recommends us to avoid one scaling in the screening function of IP as was suggested by Biersack et al. theoretically [11] and empirically [18]. Then we use the following screening function instead of Eq. (7);

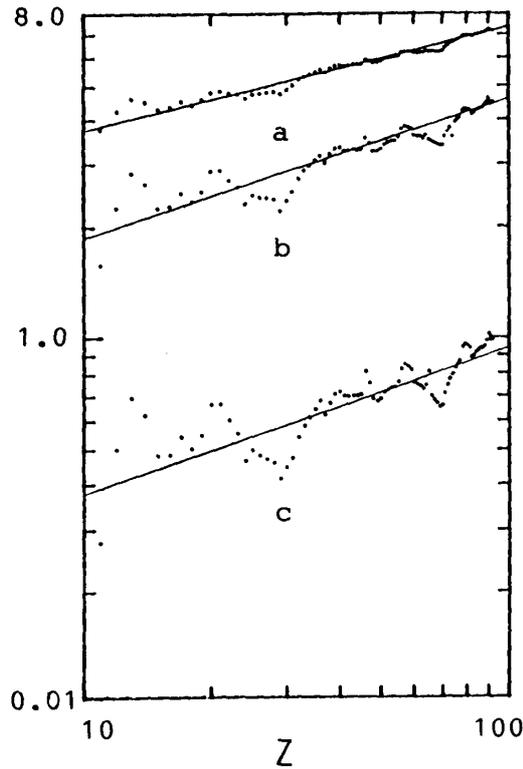


Fig. 7

Fig. 7  $Z$  dependences of (a, b, c) in Eq. (9) for respective homo-nuclear MLJ potentials are plotted against the atomic number  $Z$ . Each solid line represents the average values determined by the least square analysis, i.e., the corresponding coefficient of Eq. (8)

$$\psi(R) = \exp(-aR + bR^{1.5} - cR^2)
 \tag{9}$$

The sets of parameters (a, b, c) for respective homo-nuclear IPs are illustrated in Fig. 7 and tabulated in Table 1 with their relative standard deviation  $\sigma$ . The oscillatory tendency of the parameters of the screening function were reported [14, 15], too.

## 5. Screening function for practical use

The solid lines in Fig. 7 show the average value of respective parameters of

MLJ potentials as a function of atomic number  $Z$  by excluding the detail oscillation. These correspond to the functions of Eq. (8) one by one. Here we recommend the screening function for the practical use;

$$\psi(R) = \exp(-1.92Z^{0.289}R + 0.749Z^{0.389}R^{1.5} - 0.146Z^{0.405}R^2). \quad (10)$$

This is not universal function but practically useful.

## 6. Conclusion

We knew that our potential calculation is reasonably precise to reproduce the experimental data of the differential scattering cross section. And a new type of screening function having only three parameters was given. This screening function can be the precise IP using the parameters in Table 1 or the averaged potential using Eq. (10) for practical use, according to demands. This type can be a candidate of the good form of the screening function as seen in Appendix.

There are some Tables [6, 14, 15] to show the  $Z$  dependence in the homo-nuclear IPs, however, it seems that no systematic Table useful for wider internuclear distance has been published hitherto.

Strictly speaking the sputtering yield concerns with the low energy atomic collisions in a solid. Therefore the solid effect should be taken into the potential calculation. IP between solid-state atoms will be given [20]. Furthermore the sputtering yield can be roughly estimated only by homo-nuclear IP, however, as well as other quantities like range distribution or range straggling, the hetero-nuclear IP should be evaluated for the cases of atomic collisions in solid. The intent to construct the hetero-nuclear IP from homo-nuclear IPs is now in progress.

## Acknowledgments

The authors wish to express their appreciations to S. Enoki for helping calculation. Financial support for this work was provided by the Information Processing Center of Okayama University of Science.

## Appendix

The MLJ potential has only three parameters and is simple in the form. In order to examine the validity of this form, the existing universal potentials

such as Molière or Lenz-Jensen are expressed in the next form of MLJ potential;

$$\psi(x) = \exp(-Ax + Bx^{1.5} - Cx^2),$$

where A, B, and C are all Z independent constants. The best fit values of them are determined by the least square analysis. The results are illustrated in Fig. A associated with the original functions.

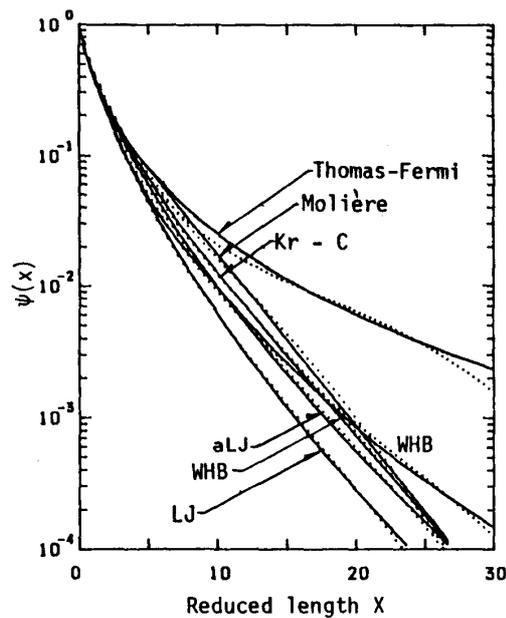


Fig. A The validity of the form of the MLJ potential of Eq. (7). The original universal potentials are shown in solid lines, while the corresponding MLJ potentials are in the dotted lines. Symbols denote the potentials, i.e., Thomas-Fermi [21], Molière [22], Kr-C and WHB [10], aLJ [1], and LJ [19].

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Table 1 Three parameters (a, b, c) in Eq. (9) for each homo-nuclear IP between gas-state atoms.  $\sigma$  denotes the relative standard deviation.

Parameters of screening function

$$U(r) = \exp(-ar + br^{1.5} - cr^2)$$

Z	a	b	c	$\sigma$	Z	a	b	c	$\sigma$
2	2.742	1.754	.6585	.01856	47	5.871	3.438	.7598	.01718
3	3.483	2.334	.6875	.02427	48	5.788	3.265	.6876	.01944
4	4.190	3.680	1.286	.02776	49	5.815	3.271	.6795	.01961
5	3.291	1.867	.5112	.004579	50	5.862	3.316	.6880	.01950
6	3.390	1.798	.4395	.04314	51	5.936	3.410	.7159	.01904
7	3.568	1.953	.4886	.003621	52	5.972	3.451	.7265	.01921
8	3.751	2.148	.5695	.003048	53	6.003	3.485	.7362	.01946
9	3.891	2.293	.6423	.003153	54	6.023	3.502	.7403	.01990
10	4.012	2.420	.7175	.003864	55	6.077	3.574	.7622	.01970
11	3.763	1.575	.2784	.009576	56	6.205	3.764	.8228	.01817
12	4.263	2.280	.5012	.004892	57	6.248	3.833	.8486	.01826
13	4.620	2.829	.6943	.006816	58	6.253	3.809	.8380	.01876
14	4.518	2.641	.6236	.003092	59	6.249	3.767	.8184	.01939
15	4.314	2.274	.4835	.009092	60	6.186	3.613	.7604	.02095
16	4.373	2.307	.4853	.009996	61	6.192	3.589	.7492	.02141
17	4.522	2.491	.5451	.008664	62	6.215	3.588	.7448	.02155
18	4.435	2.370	.5061	.01212	63	6.206	3.552	.7305	.02221
19	4.584	2.514	.5491	.01156	64	6.270	3.620	.7500	.02179
20	4.821	2.867	.6662	.008222	65	6.231	3.517	.7116	.02290
21	4.865	2.881	.6690	.008791	66	6.233	3.488	.6992	.02337
22	4.793	2.713	.6042	.01169	67	6.235	3.447	.6810	.02391
23	4.757	2.594	.5564	.01374	68	6.242	3.422	.6687	.02431
24	4.633	2.335	.4666	.01769	69	6.247	3.391	.6532	.02473
25	4.759	2.468	.5002	.01601	70	6.257	3.397	.6594	.01658
26	4.779	2.435	.4832	.01667	71	6.413	3.585	.7116	.02298
27	4.808	2.416	.4713	.01707	72	6.504	3.705	.7488	.02200
28	4.838	2.400	.4610	.01746	73	6.574	3.796	.7780	.02144
29	4.764	2.241	.4176	.02040	74	6.624	3.585	.7985	.02125
30	4.907	2.382	.4465	.01796	75	6.698	3.951	.8285	.02091
31	5.043	2.520	.4760	.01599	76	6.742	4.006	.8480	.02082
32	5.214	2.741	.5417	.01364	77	6.781	4.056	.8656	.02082
33	5.325	2.883	.5851	.01264	78	6.895	4.242	.9422	.01976
34	5.398	2.974	.6129	.01243	79	6.934	4.294	.9623	.01976
35	5.476	3.074	.6464	.01224	80	6.939	4.288	.9557	.02000
36	5.556	3.180	.6826	.01187	81	6.938	4.260	.9379	.02057
37	5.477	3.025	.6211	.01452	82	6.885	4.144	.8864	.02183
38	5.613	3.204	.6712	.01284	83	6.922	4.181	.8935	.02180
39	5.690	3.312	.7083	.01258	84	6.983	4.254	.9135	.02167
40	5.718	3.342	.7189	.01319	85	7.000	4.283	.9225	.02164
41	5.692	3.279	.6987	.01475	86	7.027	4.317	.9328	.02182
42	5.706	3.281	.6985	.01551	87	7.050	4.342	.9375	.02205
43	5.734	3.303	.7019	.01598	88	7.099	4.405	.9525	.02184
44	5.740	3.293	.7028	.01683	89	7.157	4.497	.9842	.02151
45	5.759	3.302	.7066	.01741	90	7.221	4.602	1.023	.02114
46	5.927	3.564	.8119	.01522	91	7.172	4.498	.9845	.02242
					92	7.188	4.510	.9899	.02285