

## 3 Results and Discussion

The relative values of scattering differential cross sections for each projectile at several energies were experimentally determined. In section 3.1, the background research about  $C_{60}$  and interatomic potential are described and their are used in the evaluation and discussion of some results. Section 3.2 describe about determination of the absolute differential cross section of experiments, scattering differential cross sections in  $CH_4$  and  $C_{60}$ , and moreover the results of the molecular dynamics simulations for the same collision system. In section 3.3, the extracted interatomic potentials from the measured scattering differential cross sections in  $C_{60}$  are shown, and the difference of atomic collision in  $C_{60}$  from binary collision are discussed based on the difference of the electron density distribution during atomic collision from the binary collision. In last section, Section 4, we conclude some remarkable outputs of this research.

### 3.1 Introduction

#### 3.1.1 Carbon Cluster $C_{60}$

In 1985, Kroto *et al.* [2] found a prominent  $C_{60}$  peak in the mass spectrum of laser-vaporized graphite.  $C_{60}$  is a hollow and closed-cage carbon molecule with the shape of a truncated icosahedron, like a football (see Figure 19). A fullerene is defined as a three-dimensional network of  $sp^2$  hybridized carbon atoms in which each atom is connected by a bond to exactly three neighbors [76]. The tetravalency of carbon is then satisfied by the formation of a  $\pi$  bond between each atom and one of its neighbors. The possibility that these  $\pi$  bonds might be delocalized, and so lead to an aromaticlike resonance stabilization of the molecule was, of course, one of the initial reasons for the suggestion that the buckminsterfullerene structure might be stable.

The  $C_{60}$  molecule has the shape of a truncated icosahedron with 12 pentagonal and 20 hexagonal faces (see Figure 19, Liu *et al.* 1991 [77], Hedberg *et al.* 1991 [78] and Bürgi *et al.* 1992 [79]). The diameter of

the molecule is  $d = 7.1\text{\AA}$ . There are long bonds (between a hexagon and a pentagon,  $l = 1.446\text{\AA}$ ) and short bonds (between two hexagons,  $l = 1.402\text{\AA}$ ).  $C_{60}$  form molecular solids in which the molecules are weakly bounded to each other by van der Waals forces, and it is vaporized by heating up as an isolated molecule.

The ionization energy of  $C_{60}$  is one of the important physical properties. For singly and doubly charged  $C_{60}$  ions ionization energies were measured with different methods and the values of 7.64eV for  $C_{60}$  [80] and of 11.43eV for  $C_{60}^+$  [81] are well established today. For  $C_{60}^{2+}$  the reliable ionization energies determined so far include the charge stripping result of 17.0eV by Lifshitz *et al.* [82], the corrected charge transfer bracketing results of 15.7 and 15.6eV by McElvany *et al.* [83] and Javahery *et al.* [84], respectively. In the paper of D.K. Bohme [85], many experimental values of the ionization energies of  $C_{60}$  were described in greater detail. In addition, by electron impact ionization methods, Wörgötter *et al.* had reported the appearance energies of  $C_{60-2m}^{q+}$ , that the parent charge state  $q$  is from 1 to 4 for each fragment ions of  $m=0$  to 4 [86].

### 3.1.2 The Molière Potential

The Molière potential is a simple function describing interatomic potentials which includes electronic screening effects based on the Thomas-Fermi statistical model of the atom [57]. The screening function  $\chi_M(x)$  which is an approximation to the Thomas-Fermi screening functions (see Appendix A) represented by Molière [60] is

$$\chi_M(x) = 0.35e^{-0.3x} + 0.55e^{-1.2x} + 0.10e^{-6.0x}, \quad (23)$$

as depicted in Figure 20. Molière's expression is only an approximation to the Thomas-Fermi screening function. To insert Molière's screening function, Eqn. (23), into the Thomas-Fermi equation, Eqn.(48), we checked the applicable range of the Molière screening function. The results are shown in Figure 21. For ranges less than  $x \sim 0.1$ , the accuracy decreases. Therefore,

the electron density  $n_e(r)$  will not be described exactly; however, since the boundary condition  $\chi(0) = 0$  is satisfied, the potential described by Molière closely approximates the real potential.

The the two-center Thomas-Fermi problem was considered by Firsov, and evolved two-body potential of the general form,

$$V(r) = \frac{Z_1 Z_2 e^2}{r} \chi(r/a_F). \quad (24)$$

The  $a_F$  is the converted Thomas-Fermi screening radius, Eqn. (46), for the interaction between the two atoms of atomic numbers  $Z_1$  and  $Z_2$ , suggested by Firsov as follows,

$$a_F = \frac{0.88534 a_0}{Z_{eff}^{1/3}} \quad (25)$$

where  $Z_{eff}$  is the effective charge number in the interaction of two unlike atoms. That is to say, the interatomic potential between two atoms is represented as a one body potential (reduced potential) with a single effective atomic number,  $Z_{eff}$ .  $Z_{eff}$  is estimated by a minimization of the total energy of the two-atom system which includes the electron kinetic energies, the Coulomb interactions between the electrons and the nuclei and the interactions between the electrons. Firsov tried numerical calculations for several collision systems, and finally presented as his two-body interatomic potential based on Thomas-Fermi theory, the potential described by Eqns. (24) and (25) with  $Z_{eff}$  as follows

$$Z_{eff} = \left( \sqrt{Z_1} + \sqrt{Z_2} \right)^2, \quad (26)$$

valid in the range  $r \leq 1 \text{ \AA}$ .

From the 1950s to the 1960s many experiments on the scattering of ions and neutral atom beams by gas phase atom targets at different energies with a variety of target and incident atom combinations were performed. G. H. Lane and E. Everhart compared the potential deduced from experimental data on ion-atom collisions with the theoretical potential suggested by Firsov

[87]. The ion-atom combinations studied included Ar<sup>+</sup> on Ar, Ne<sup>+</sup> on Ar, Ne<sup>+</sup> on Ne, He<sup>+</sup> on Ar, He<sup>+</sup> on Ne, and He<sup>+</sup> on He, using differential cross section measurements by Fuls *et al.* [88] and Jones *et al.* [89] made at 25, 50 and 100 keV. These data were analyzed using equations developed by Firsov. The potential energies are positive, in the range of one to sixty thousand electron volts, and correspond to ion-atom separations of a small fraction of an angstrom. The resultant potential energy curves were compared with a function derived by Firsov from a statistical model, and they were found to fit fairly well.

To compare Firsov's screening radius, Eqn. (25), with interatomic potentials extracted from experimental results, especially at large distances, the equation for the screening radius, Eqn. (25), was corrected by O'Connor and MacDonald [63] as follows,

$$a_c = \frac{0.88534a_0}{(\sqrt{Z_1} + \sqrt{Z_2})^{2/3}} f(Z_1, Z_2) \quad (27)$$

where  $f(Z_1, Z_2)$  is the correction factor determined by least squares fitting with the experimental results as follows,

$$f(Z_1, Z_2) = 0.54 + 0.045(\sqrt{Z_1} + \sqrt{Z_2}) \quad (28)$$

This correction is especially effective at a large distance in collisions between two atoms. The values of  $a_F$  and  $a_c$  for the collision in our experiments are shown in Table 3.

In our study, the interatomic potential represented by, Eqns. (23), (24) and (27) were used, that is

$$V_M(r) = \frac{Z_1 Z_2 e^2}{r} \chi_M(r/a_c) \quad (29)$$

This is usually called the Molière potential. Using theoretical and empirical expressions, Molière potential accounts well for the interatomic potential at potential energies from several eV to several keV. In fact, the higher the

energy, the better the approximation because it closes the pure Coulomb potential.

A classical calculation of the differential cross section for scattering is valid when the deBroglie wavelength  $\lambda$  of the incident particle is negligible compared with any significant dimension of the scattering center [90]. This condition requires that  $\lambda$  be much smaller than the screening radius  $a$ , and also much smaller than the collision impact parameter  $b$ . For the present experiments, the screening radii are shown in Table 3, and it is estimated that the impact parameters are larger than about  $0.1\text{\AA}$  for any kind of noble gas atom and for incident energies within the range of our measurements. The de Broglie wavelengths were calculated using the equation  $\lambda = h/mv = h/\sqrt{2m_1 E_0}$ , and are shown in Table 4. Since these values are much smaller than the values of  $a$  and  $b$ , all conditions for the validity of a classical solution are satisfied in the present studies.

The differential cross sections of elastic collision of atoms at a few keV are calculated using the Molière potential by the methods of classical dynamics as follows,

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin \theta} \left| \frac{db}{d\theta} \right| \quad (30)$$

where  $b$  is the impact parameter of the incident atom and the target, and  $\theta$  is the deflection angle of the particles. The relation between  $b$  and  $\theta$  is given by

$$\theta = \pi - 2 \int_{r_m}^{\infty} \frac{b}{r^2 \sqrt{1 - \frac{b^2}{r^2} - \frac{V(r)}{E}}} dr \quad (31)$$

where  $r$  is the distance between the two atoms,  $E$  is the collision energy,  $V(r)$  is the interatomic potential and  $r_m$  is the distance of closest approach between the incident atom and the target. The  $r_m$  is a solution of the equation

$$1 - \frac{b^2}{r_m^2} - \frac{V(r_m)}{E} = 0 \quad (32)$$

which includes the interatomic potential, and which for our experiments is calculated using the Molière potential as a function of the scattering angles.

Plots of  $r_m$  as a function of the scattering angle are shown in Figure 22. In order to obtain the scattering differential cross section from any interatomic potentials in Eqn. (30) as a function of the scattering angle alone, Eqn. (31) was solved numerically for  $b$  as a function  $\theta$ . Inversely, the interatomic potential is extracted using these equations from a curve of scattering differential cross sections.

## 3.2 Experimental and Theoretical Results

### 3.2.1 Determination of Absolute Quantity of the Cross Sections

In order to determine the absolute quantities of relative differential cross sections, by a simple method, the intensity of the incident atoms, the target density and the absolute detector efficiency are required. But, in this experiment, determining the absolute value of the target density was difficult. So we had to normalize the measured relative cross sections of a evident atomic collision in physically with the theoretical calculation of cross section.

The absolute cross sections were evaluated based on the assumption that the quasi-elastic scattering of a  $\text{He}^+$  ion on a  $\text{C}_{60}$  at a few keV should not be affected so much by the boundary conditions of the carbon atom embedded in the  $\text{C}_{60}$  cage because a calculation based on the Molière potential showed that, under the kinematics of the present study, the elastic scattering of a  $\text{He}^+$  ion on an isolated carbon atom occurs mainly in a small region of radius less than  $0.1\text{\AA}$  around the carbon atom, which is one order of magnitude smaller than  $1.40\text{\AA}$  average distance between the two nearest carbon atoms shared by adjacent. This allows us to calculate the theoretical differential cross section with the Molière potential for the  $\text{He}^+$  (4 keV) +  $\text{C}_{60}$  collisions are used to normalize the corresponding measured relative differential cross section, which in turn allows us to normalize the relative differential cross section for the other noble gas +  $\text{C}_{60}$  collision through Eqn. 10.

Actually, we had done least squares fitting the so-obtained relative cross sections of  $\text{He}^+$  +  $\text{C}_{60}$  with the cross section of theoretical calculation

using Moliere potential. The evaluated  $\chi^2$  value was 16.77, and the consistency is well established in Figure 24. At the same time, we obtained the overall normalization factor which was applicable for all the cross sections. In other words, it has been found that we can measure the absolute cross sections for any species of noble gas atoms interacting with  $C_{60}$  by reference to the experimental yield of the quasi-elastic scattering of  $He^+$  on a  $C_{60}$ . The scaling for normalizing measurements on the  $CH_4$  target was deduced by the same method, and the results are shown in Figure 23.

### 3.2.2 Scattering Differential Cross Sections in $CH_4$

Fig. 25 shows the differential cross sections for collisions of several kinds of noble gas ions with carbon in  $CH_4$  targets. The absolute values of experimental results are indicated by the symbols. The calculations using a pure Coulomb potential, namely the Rutherford cross sections, are larger than the experimental results. Obviously, the electronic screening effect needs to be incorporated into the interatomic potential. The solid curves are the calculations using the Molière potential which include screening effects, and they fit the experimental results very well collectively, not only the magnitude of the experimental results, but also the shape of the angular distribution.

Figure 26 shows, the differential cross sections for argon and carbon for incident energies from 4.2 keV to 10 keV. In these experiments calculations using the Molière potential perfectly represent the experimental results.

The collision interaction between the noble gas ions and carbon are described by the Molière potential which is a two-body interatomic potential with electronic screening effects in spite of the fact that  $CH_4$  is a compound molecule of carbon and hydrogen. It is clear that the influence of the hydrogen on the collision of the noble gas ions and carbon is negligibly small not only for the case of  $He$  (4 keV) +  $C$ , but even when the distance of closest approach, which is shown in Figure 22, is quite large as in the case of a collision between  $Ar$  and carbon ( $r_m \sim 0.3\text{\AA}$ ) at 4.2 keV. The consistency between the experimentally and theoretically derived scattering differential cross sections

confirms the reliability of the experimental setup and the analysis methods.

### 3.2.3 Scattering Differential Cross Sections in $C_{60}$

For  $C_{60}$ , the experimental and theoretical results are shown in Figure 27. There are several remarkable points to be considered. First, it should be noted that the calculation fits the measured differential cross sections of  $He^+$  on  $C_{60}$  at 4 keV very well. Since the distance of closest approach ( $0.05\text{\AA} \sim 0.1\text{\AA}$ ) is one order smaller than the distance between adjacent carbon atoms in  $C_{60}$  ( $\sim 1.4\text{\AA}$ ) for this case as shown in Figure 22, any effects due to neighboring carbon atoms are negligible. Therefore we can conclude a pure two body collision occurred.

Second, we can observe the serious discrepancy between the calculated and the measured differential cross sections of other ions on  $C_{60}$ . The experimental values are smaller than the theoretical ones. In other words, the measured differential cross sections are much lower than those expected for isolated carbon atoms. It seems that a screening effect is occurring.

Third, the observed discrepancy is enhanced at the forward scattering angles. In other words the discrepancy becomes larger for larger impact parameters. This fact seems to indicate the presence of some many body effects in atomic collisions in a many body system such as  $C_{60}$ . If it were only a difference of magnitude, it would be possible to fit the calculation to measurements by changing the screening radius, but this can not be done. The difference in shape of the two curves for the scattering differential cross section must be the result of some unknown, significant collision mechanisms.

In Figure 28, the energy dependence of the scattering differential cross section from 4.2 keV to 10 keV is shown. The larger the collision energy, the smaller the discrepancies at forward angles. This suggests, the discrepancies may depend upon the interatomic distance between the collision atoms.

Shown in Figure 29, the suppression factor calculated by dividing the measured differential cross sections by the theoretical ones, as a function of the energy of the recoiling carbon calculated from TOF measurements. The



tendencies of the suppression for Ne and Xe were different from each other. The recoil energy of the carbon was the same for each scattering angle, as mentioned in Section 2.6. As a result, the suppressions were independent of the recoil carbon energy. Therefore, secondary collision effects of the recoiled carbon in the  $C_{60}$  has little relation to the suppression results, probably.

Two reasons for this discrepancy have been considered. The first is the effects of multiple atomic collisions in  $C_{60}$ . Since the kinetic energy after collision is consistent with the kinematics of an elastic two-body collision, it is safe to assume multi-collision effects were small.

The second reason is the difference of the interatomic potentials between atomic collisions with  $C_{60}$  and with isolated atoms. In other words, since the interatomic potential is strongly influenced by electronic screening effects, the results of these experiments indicate a difference of electron density between the two types of collisions.

### 3.2.4 Molecular Dynamics Simulation

In order to explore some multi-collision effects, the Molecular Dynamics (MD) simulations (computer simulations) of atomic collisions for noble gas atoms into  $C_{60}$  molecule with the same kinetic energy as our experiments were performed by Muramoto and Yamamura in 1998 [91]. In these simulations the multiple collision effects based on the Molière potential were as follows:

1. interaction of the incident atom with several carbons at the same time
2. collision of the incident atom with different carbons at different times
3. collision of the primary recoiling carbon with other carbon atoms
4. collision of the incident atom with a single carbon at different positions, e.g., center or off-center
5. shadowing effect of the carbons in the front surface of the  $C_{60}$  (cf. [92])

The interatomic potential, used in the simulations, between noble gas atoms and carbons was a Molière potential, and that between the carbon atoms was a hybrid potential which was a combination of the Molière potential and the Tersoff potential [93, 94]. The Molière potential dominates when the distance between carbons is less than 1 Å and the Tersoff potential dominates for more long ranges. The Tersoff potential is important in stabilizing the molecular structure of the C<sub>60</sub>, and it hardly influences the knock-out. The output of this simulation was the distribution of inverse velocity after collision for laboratory angles at steps of 5° with an ambiguity of ±2.5°. The time of flight spectra are shown in Figure 30. An interesting feature of the results is the presence of a few quasi inelastic carbons in the peaks for large angles. In order to make clear the multi-collision effects, we compared the scattering differential cross section derived from the simulation with the theoretical calculated differential cross section using the two-body Molière potential. In Figure 31 the scattering differential cross sections analyzed from the results of the MD simulation are shown. For the collision of Ne (3.2 keV) with carbon the results of the MD simulation agree with the two-body calculation using the Molière potential. Therefore, it is concluded that a collision of the primary recoiled carbon with other carbon atoms in a C<sub>60</sub> is a rare event. The magnitude of the cross sections were verified by the agreement between the MD simulation and the Molière calculation. In conclusion, multiple collision effects are rare in knock-out scattering for large scattering angles.

But, in the large impact parameter collisions, multiple collisions for incident atoms are observed both in experiments and simulations. In Figure 32, TOF spectra are shown from experiments with the CH<sub>4</sub>, from experiments with C<sub>60</sub> and from the MD simulation for Ar atoms at an energy of 4.2 keV. For the CH<sub>4</sub> and C<sub>60</sub> experiments the solid angles for detection are the same within ±1.4°. In the time of flight spectrum for the CH<sub>4</sub> experiment, there are no scattered argon peaks, but they appear it is shown in measurements for the C<sub>60</sub> and in the simulation too, therefore, we can identify the large peak is the experimental TOF spectrum as an argon peak. If these multiple

collisions which produce the Ar peak were two-step collisions of Ar for  $10^\circ + 10^\circ$  in the laboratory frame, the yield of the recoiling carbons would be enhanced around  $40^\circ$  in the center of mass frame. However, in the experiment the yields are suppressed. The yield ratio of scattered Ar to carbon, including multi-collisions, is smaller in the experiments than in the simulation. The yield ratio, C:Ar, at  $\theta_L = 20^\circ$  is 1:9.3 and 1:7.9 for the MD simulation and the experiment, respectively. This suggest that in the experiments the interaction of Ar with carbon is a little weaker than the Molière potential would predict.

### 3.3 Data Analysis

#### 3.3.1 Free Parameter Optimization

Since the multiple collision effects are negligible, we assumed that the difference between the scattering differential cross sections for  $C_{60}$  and for an isolated carbon is due to a difference between the interatomic potentials in the two cases, caused by a difference in the electron density distributions. Therefore, we tried to find a model for the interatomic potential for each kind of incident atom.

We perform to find a optimal interatomic function for atomic collisions with  $C_{60}$  by numerical free parameter optimization methods, using a discrete function with several number of free parameters working to change the potential curve freely, as follows,

$$V(r_i) = k_i \cdot V_M(r_i) \quad (33)$$

where  $k_i$  are independent parameters at the interatomic distance with a space of  $0.05\text{\AA}$ , i.e.,  $r_i$  is atomic distance  $r_i = \dots 0.10, 0.15, 0.20 \dots$ , and this is shown in Figure 33. The initial value of all parameters  $k_i$  were set to 1. The differential cross section was calculated by classical dynamics using the potential which provided by the spline interpolation of  $V(r_i)$ , and the least squares fitting was performed at the differential cross section derived from the

interpolated  $V(r_i)$  to the measured cross sections. As a result, a optimized function were determined by the minimum search algorithm.

In Figure 34 the results of optimized parameters  $k_i$  are shown, that is,  $k_i$  as a function of the atomic distance  $r$ . These results indicate that a additional screening function and that it is well modelled by a Woods-Saxon type function.

### 3.3.2 Additional Screening Function $S(r; a_1, a_2, a_3)$

From the result of previous section, the effective potential was factorized as

$$V_{MB}(r) = S(r) \times V_M(r) \quad (34)$$

The function  $S(r)$  was approximated by a Woods-Saxon type function with three parameters as follows

$$S(r) = a_1 + \frac{1 - a_1}{1 + \exp \{(r - a_2)/a_3\}}, \quad (35)$$

where  $a_1$  is an offset,  $a_2$  indicates the overall width of additional screening function  $S(r)$ , and  $a_3$  indicates width of falloff of  $S(r)$ .

To obtain the best value for the parameters,  $a_1$ ,  $a_2$  and  $a_3$ , we performed a least squares fit at the scattering differential cross sections derived from  $S(r; a_1, a_2, a_3)$  to the measured cross sections.

First, the  $S(r)$  function was determined for Ar and  $C_{60}$  using the measurements at 4.2, 6.0, 8.1 and 10.0 keV at the same time. In Figure 35 the differential cross sections derived from the estimated  $V_{MB}$  function agree well with the experimental results for all energies. From the results of free parameter optimizations shown in Figure 34, the offset  $a_1$  is almost the same for the three incident atomic species. Therefore,  $a_1$  is fixed to the value for Ar. Next the parameters  $a_2$  and  $a_3$  were determined for the Ne and Xe collisions. In Figure 36 the fitted differential cross section curves are very good approximations for all the measured angles. The values of the parameters are shown in Table 5.

In Figure 37 the parameter  $a_2$  as a function of  $Z_1$  is shown. The  $a_2$  parameter becomes larger as the atomic number increases. The overall width of the additional screening,  $a_2$ , depends strongly on the atomic number of the noble gas ion. It seems to be related to the magnitude of the potential between the noble gas atom and the carbon. In Figure 38, the  $Z_1$  dependence of  $a_3$  is shown. The falloff width of  $S(r)$ ,  $a_3$ , tends to become narrower as  $Z_1$  increases.

In Figures 39, 40 and 41, for Ne, Ar and Xe, the extracted, or new interatomic potential, the Molière potential, which is a pure two-body interatomic potential; and the pure Coulomb potential are shown. Again, we can see the anomalously strong screening effects in atomic collisions with  $C_{60}$ , and that they are surprisingly well represented by a simple Woods-Saxon type function with three parameters.

In Figure 42, the additional screening function is plotted as a function of the corresponding Molière potential for each noble gas. The three curves intersect at a common point at which the Molière potential is  $\sim 1300$  eV and  $r = a_2$ . This implies that there is a scaling rule for the additional screening function. And, the similarity and trend of the slope of the curves suggest a dependence of the slope on the atomic number of the incident atoms.

### 3.3.3 Electron Density Distribution of Reduced Atom

The interatomic potential between noble gas atoms and a carbon in  $C_{60}$  are determined by Eqns. (34) and (35) with the parameters in Table 5 and Eqn. (29). The electron density distributions of the reduced atom were deduced using Poisson's equation, Eqn. (41), from the interatomic potential functions, i.e.,

$$|n_e(r)| = \frac{1}{4\pi e} \nabla^2 V(r) \quad (36)$$

The Molière potential and the new interatomic function  $V_{MB}(r)$  are easily differentiated analytically. We plotted the electron density distribution curves both of the  $V_{MB}(r)$  and  $V_M(r)$  in Figure 43. The experimental curves differ from the Molière potential more and more as the reduced atomic number

$Z_{eff}$  increases. The value for the electron densities are infinity at  $r = 0$  in the figure, however, it should vanish at  $r = 0$ , i.e., at the center of the nuclei. This error probably comes from the low accuracy of Molière's screening function, Eqn. (23), as opposed to the Thomas-Fermi screening function, Eqn. (48), near  $r = 0$  (see Figure 21). The estimated value of the electron density in the Xe + C<sub>60</sub> system becomes negative at around  $r = 0.33\text{Å}$ . This inaccuracy most likely reflects an invalid extrapolation of the results from the experimental data for  $r > 0.4\text{Å}$  to  $r < 0.4\text{Å}$ . Recall that the distance of closest approach is equal to about  $0.4\text{Å}$  in this experiment. But, it also could be the result of other effects besides electronic screening, for example, a weak interaction with neighboring carbons (weak multi-collisions). In any event, in the future the differential cross sections should be measured for smaller distances between the incident particle of Xe and the target of C.

The electron density distributions are not the real densities between two atoms, but for only the reduced-charge atom for a one-body problem. However, the electron density must naturally be modified between two atoms influenced by the environment of the C<sub>60</sub>. To clearly show in what region and to what extent the electron density is modified, the ratio of the experimental density to the Molière density is depicted in Figure 44. The magnitude of the modification factor increases with the charge number of the incident atom, suggesting that the capacity for modification of the electron density is larger for atoms with larger atomic numbers.

The total electronic charge is calculated by

$$Q = \int_0^{\infty} n_e(r) \cdot 4\pi r^2 dr. \quad (37)$$

The integrand function is 0 at  $r = 0$  and  $r = \infty$ . Even with the negative density values, total integral is positive for the Xe-C case. The results are shown in Table 6. The results using the Molière potential are exactly the  $Z_{eff}$ . The experimental potential gives almost the same results. Therefore, the total charge is conserved throughout the collision reaction on the average.

### 3.4 Discussion

It is probable that the crystal-like structure of  $C_{60}$  is responsible for the observed anomalously strong screening effect, which wasn't observed in the  $CH_4$  experiments. The atomic number dependence of the overall width of the additional screening function,  $a_2$ , and the width of its falloff,  $a_3$ , suggests that the many body of  $C_{60}$  greatly structure affects the approaching noble gas ions.

The structural differences between  $CH_4$  and  $C_{60}$  lead to a considerable difference between interatomic potentials. We believe these are three basic structural differences that account for the differences in the potentials. The first concerns the distribution of the 60  $\pi$  electrons in  $C_{60}$ . The Second concerns the boundary conditions of the potential between the noble gas atom and the carbons in the crystal structure of the  $C_{60}$ . The third difference is the new additional electronic screening effect by the electrons restricted around the many body nuclei when the noble gas atom breaks into between the  $C_{60}$  cage.

The third difference may be the most important one in considerations of many body effects. The average velocity of electrons in the noble gas atoms and carbons described by the Thomas-Fermi model are faster by several orders of magnitude than the ion projectiles (see Figure 45). When a many body Coulomb force is exerted between the carbon nuclei and the nucleus of the embedded noble gas atom, it is highly likely that the electron density distribution different from that determined by the Coulomb field of two nuclei, studied by Firsov.

Furthermore the "scaling rule" of the additional screening function suggests that some important physical principle may be revealed from further studies of this phenomenon. However, the additional screening effect was not seen in the experiments with  $He^+$  (4keV) + C in  $C_{60}$  even when the interatomic potential  $V_M(r)$  was several hundred eV. We think this is because the modification of the electron density distribution is restricted to a relatively large distance from the nucleus, so the  $1s$  electron shell at the

He and C atom are not modified.

The electron density distribution of the reduced atom with atomic number  $Z_{eff}$  was shown in Section 3.3.3. The difference between the electron density distribution in atomic collisions in  $C_{60}$  from that in 2-body collisions was made clear. Even if the results don't indicate the real electron density distribution between the noble gas atom and the carbon atom, they give some information on atomic collisions at a few keV in the many body system.