Many Body Effects in Atomic Scattering of Ions by Individual Carbons in $C_{60}$
at a Few keV

Takashi MIURA

A dissertation submitted to the Doctoral Program in Physics, the University of Tsukuba
in partial fulfillment of the requirements for the degree of Doctor of Philosophy (Science)

February, 1999
Abstract

The collision dynamics of the noble gas atoms He, Ne, Ar, and Xe on C_{60} at incident energies from 3.2 keV to 10 keV have been studied. We measured the differential cross sections of quasi-elastic collisions between the noble gas atoms and a carbon in C_{60}. For comparison, we performed similar experiments on CH_4. In order to evaluate the experimental results, theoretical calculations of the differential cross sections for binary collisions between the noble gas atoms and a carbon atom using the Molière potential, which describes various types of binary atomic collisions phenomenologically, were performed. The results of the calculations agree with the experimental results for CH_4. On the other hand, the results for C_{60} are much more suppressed than those obtained for isolated carbon atoms, and the discrepancy becomes larger at forward angles. We attribute this suppression to an anomalously strong screening effect. The additional screening factors have been evaluated numerically through a least-squares fitting to the measured cross sections. The resulting screening factors seem to be represented well by simple Woods-Saxon type functions with three parameters. Two parameters, which define the function's overall width and the width of its falloff, are variable, while the third is a constant common to all collisions. Furthermore, when the additional screening functions were “scaled” by the binary atomic potential, the Molière potential, they were found to be independent of the atomic number of the noble gas atoms. This additional screening effect is considerably influenced by the electron density distribution in the many body system consisting of the carbon atoms of the C_{60} and the noble gas atom.
Contents

1 Introduction .......................................................... 1

2 Experiment .............................................................. 9
  2.1 Source of Noble Gas Ions ..................................... 9
  2.2 Beam Pulsing System .......................................... 9
  2.3 Supersonic Molecular Beam Source for CH₄ Gas Target .... 10
  2.4 Effusive Molecular Beam Source for C₆₀ Gas Target .......... 12
  2.5 Particle Detectors ............................................. 14
  2.6 Time of Flight Measurements .................................. 15
  2.7 Effective Solid Angle of the Detector ......................... 16
  2.8 Extraction of the Differential Cross Section .................. 18

3 Results and Discussion ............................................... 20
  3.1 Introduction ................................................... 20
    3.1.1 Carbon Cluster C₆₀ ...................................... 20
    3.1.2 The Molière Potential .................................... 21
  3.2 Experimental and Theoretical Results ......................... 25
    3.2.1 Determination of Absolute Quantity of the Cross Sections 25
    3.2.2 Scattering Differential Cross Sections in CH₄ ........... 26
    3.2.3 Scattering Differential Cross Sections in C₆₀ .......... 27
    3.2.4 Molecular Dynamics Simulation .......................... 28
  3.3 Data Analysis .................................................. 30
    3.3.1 Free Parameter Optimization ............................. 30
    3.3.2 Additional Screening Function S(r; a₁, a₂, a₃) .......... 31
    3.3.3 Electron Density Distribution of Reduced Atom .......... 32
  3.4 Discussion ..................................................... 34

4 Conclusion ............................................................ 36

A Thomas-Fermi Model ..................................................... 38