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TARGET THICKNESS DEPENDENCE OF Cu K X-RAY PRODUCTION
FOR IONS MOVING IN THIN SOLID Cu TARGETS

DISSERTATION

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Measurements of the target thickness dependence of the target x-ray production yield for incident fast heavy ions are reported for thin solid Cu targets as a function of both incident projectile atomic number and energy. The incident ions were F, Al, Si, S, and Cl. The charge state of the incident ions was varied in each case to study the target x-ray production for projectiles which had an initial charge state, q , of $q = Z_1$, $q = Z_1 - 1$, and $q < Z_1 - 1$ for F, Al, Si, and S ions and $q = Z_1 - 1$ and $q < Z_1 - 1$ for Cl ions. The target thicknesses ranged from 2 to 183 $\mu\text{g}/\text{cm}^2$. In each case the Cu K x-ray yield exhibits a complex exponential dependence on target thickness. A two-component model which includes contributions to the target x-ray production due to ions with 0 and 1 K vacancies and a three-component model which includes contributions due to ions with 0, 1, and 2 K vacancies are developed to describe the observed target K x-ray yields. The two-component model for the Cl data and the three-component model for the F, Al, Si, S, and Cl data are fit to the individual data for each projectile, and the cross sections for both the target and projectile are determined. The fits to the target x-ray data give a systematic

representation of the processes involved in x-ray production
for fast heavy ions incident on thin solid targets.

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CHAPTER I

INTRODUCTION

The questions associated with processes involving interactions of high velocity ions moving in matter are of great importance. The physics to be obtained from studies involving atomic systems is related to fundamental interactions of highly ionized or excited atomic systems. Such systems are important to the understanding of stellar atmospheres, the dynamics and energy exchange processes of high temperature plasmas such as in the controlled thermonuclear fusion processes, the role of ion-atom collisions in radiation damage and material modification, and the viability of the approach to describing the inner shells of atoms which employ a variety of simplifying assumptions in order to make the calculations for such systems tractable.

Because of the need for accurate data and descriptions of ion-atom collisions there has been in the last decade, a renewed interest in the study of inner shell ionization associated with the impact of high velocity ions. The availability of improved detection technology for use in ion-atom collisions resulting in atomic excitations and the use of accelerator facilities previously dedicated to nuclear physics studies has resulted in major advancements

in the understanding of ion-atom collisions. While there is no specific definition of the type of incident ions used in such studies, they can generally be classified as light ions (e.g. H, He. .) or heavy ions (e.g. F, Cl, Ar. .). This classification scheme must necessarily take into consideration the relative atomic numbers of the projectile (Z_1) and the target (Z_2). Generally the theoretical developments have treated the case of ionization by light ions ($Z_1/Z_2 \ll 1$) by considerations based upon direct Coulomb ionization. The plane wave Born approximation (PWBA),¹ binary encounter approximation (BEA),² and semiclassical approximation (SCA)³ were developed on this basis as discussed in Appendix A. Comparisons of these three theories to K- and L-shell ionization cross sections for H ions over a large range of target atomic numbers and incident ion energies⁴ have established that the general features of the experimental data are predicted.

A fundamental feature of the direct-Coulomb theories of inner shell ionization is that the ionization cross sections should scale as Z_1^2 (See Appendix A). Experimental investigations using He and Li ions⁵⁻⁹ to study both K- and L-shell ionization have shown that the cross sections do not scale as Z_1^2 . Work by Basbas, Brandt, and Laubert¹⁰ had previously shown that considerations of the effects of perturbations in the target electron binding energy and deviations from a straight line

trajectory for the projectile gave improved agreement between experimental data and theory for K-shell ionization in the case of H on Al. Their work was based upon the inclusion of binding energy and Coulomb deflection corrections as perturbations to the PWBA. Calculations for ionization by He and Li ions which include these effects (PWBABC) gave improved agreement with target K-shell cross section data for systems like He on Cu and Li on Cu.

Experiments which have extended the incident atomic numbers to include C, N, O, F, Si, S, and Cl have been reported.¹¹⁻¹⁶ The general experimental approach used by the groups involved has been to employ the techniques associated with the studies of inner shell ionization by light ions in thin solid targets. McDaniel and Duggan¹³ have reported K x-ray cross section data for targets of Ti, Ni, Ge, and Rb ranging in target thickness from 5- to 100- $\mu\text{g}/\text{cm}^2$ for incident ions ranging from H to Cl. Tserruya et al.¹⁴ have reported results for S ions on targets of Mn, Ni, Cu, Zn, and Ge having thicknesses less than 100 $\mu\text{g}/\text{cm}^2$. Comparisons of these data to theory have been made using the PWBA, PWBABC, and PWBABC with additional corrections for energy polarization¹³ and relativistic effects.^{13,17} Additional comparisons¹⁴ have been made to SCA, BEA, and a vacancy sharing model proposed by Meyerhof.¹⁸ Measurements have shown that

the inclusion of the above perturbations to the PWBA gives improved agreement for the light ions (H, He, Li, C, and N). The same type of theoretical calculations result in a significant reduction in the magnitude of the calculated K-shell cross sections for heavy incident ions (F, Si, S, and Cl). The systematics of the disagreement between the calculations and the data for K-shell ionization for heavy ions show that the PWBABC underestimates the measured cross sections by factors ranging from an order of 2 to 100 depending upon the ion velocity and the target atomic number. In a case such as Cl on Ti¹³ the PWBA predictions are within a factor of 2 of the reported cross section measured for a thin solid Ti target while the PWBABC calculations are a factor of ~ 100 below the measured x-ray production cross section. Measurements for Cl on Rb¹³ show the opposite agreement with the PWBA being a factor of ~ 30 larger than the measured target K-shell cross section and the PWBABC predictions being a factor of 4 smaller than the reported cross section.

Such variations in the comparisons of direct Coulomb ionization predictions and experimental data for heavy ions on thin solid targets suggest that there are additional considerations having important theoretical and experimental consequences for understanding the processes involved. Measurements of K-shell x-ray production for symmetric collisions in the cases of Al-Al and Ni-Ni

have been reported for thin solid targets by Laubert et al.¹⁹ Their work covers the energy range of 0.5 - 40.0 MeV for Al-Al and 10-63 MeV for Ni-Ni collisions. The work was performed to cover the energy regions wherein the transition from predominately quasimolecular excitation to direct Coulomb excitation should occur (See Appendix A). Comparisons of their data to scaled deuteron-deuteron cross section were made using the procedure reported by Briggs and Macek.²⁰ Additional calculations for the PWBA and modified PWBA were also reported.¹⁹ The data for Al-Al were predicted by the quasimolecular calculation for incident energies below 3 MeV. However, above 3 MeV the data began to rise above the quasimolecular predictions with increasing ion energy approaching the PWBA predictions. In the case of Ni-Ni the data for the K-shell x-ray production cross section were not represented by the theoretical calculations.

When taken in total the reported measurements and interpretations of target x-ray cross section data for heavy ions on thin solid targets have not provided to date the information required to allow adequate evaluation of the theoretical models for inner shell ionization by heavy ions incident at high velocities. Given that the state of comparison between theory and experiment requires improvement, where can other effects that may be of primary importance be brought into consideration? One important contribution may reside in the effects of the K-shell vacancy configurations of the

projectile in the solid. Results reported by Winter et al.²¹ and Mowat et al.²² for heavy ions incident upon gas targets under single collision conditions has suggested a charge dependent effect for the target x-ray production cross sections. The target x-ray production is observed to increase with the increasing charge state of the projectile at a fixed incident energy. Part of the observed increase may be associated with a changing fluorescence yield in the target atom. However, there is a larger enhancement in the target x-ray yield for hydrogen-like and bare projectiles. This suggests that the existence of K vacancies in the projectile is involved in the target K-shell ionization process.

A model to account for such variations seen for O ions on solid Al targets has been proposed by Brandt et al.²³ This model is based upon the dynamic screening of the projectile charge by the target electrons. In this model the target electrons are treated as an electron gas which responds to the presence of the high velocity ion through the ion-electron interaction. The effect of the solid target on the ionization process is assumed to be associated with a dynamic screening rate, λ . The effective charge of the ion is given by

$$q_1(x) = q_1(0) e^{-\lambda v_1/x} + q_1(\infty) (1 - e^{-\lambda v_1/x}) ,$$

where $q_1(0)$ and $q_1(\infty)$ are the incident and equilibrium charges, respectively. The ionization cross section for the

target is approximated by

$$\sigma_I(x) = \frac{\sigma_I}{T Z_1^2} \int_0^T q_1^2(x) dx .$$

The change in the cross section is thus treated as arising solely from an effective screened projectile charge. In the limit of a vanishingly thin target the ratio of ionization cross sections for two incident charge states q_1 and q_1' is then proportional to $(q_1/q_1')^2$. In a projectile-target system such as Cl ions on Cu, the dynamic screening model predicts that the ratio of K-shell ionization cross sections for incident Cl ions in charge states 16+ and 14+ is 1.3. It will be shown in the present work that this prediction is not correct, as the measured ratio of target K x-ray production cross sections (hence, ionization cross section) for Cl on Cu is 8.1. In the dynamic screening model the screening rate is assumed to depend on the plasma frequency of the target electrons, and thus it is independent of the incident ion species. The bound electrons of the target are assumed to not contribute to the processes which may effect the inner shell ionization mechanisms for heavy ions moving at high velocities in solid targets. While there may be a range of validity for such considerations at low incident ion velocities, the experimental results presented in the present work cannot be described by assuming that dynamic screening is of major importance at higher velocities.

In the dense medium of a solid target the vacancy production and quenching interactions will govern the number of K vacancies in the projectile as it traverses the target. Hence, the existence of fractions of the incident ion beam with one or two K vacancies can be reflected in the target x-ray production cross section. In order to observe such effects two important criteria have to be met: (1) there has to be strong coupling between the K vacancies of the projectile and the target K-shell electrons to give rise to enhanced target K-shell ionization, and (2) there has to exist strong coupling of the projectile K shell to the target medium in order to create and/or destroy projectile K-vacancy configurations.

Allison²⁴ discussed the methods of describing the role of charge-changing collisions for H and He ions moving in gases and solids. Equations were derived which predict the charge states for two- and three-component systems as a function of target thickness. Betz et al.²⁵ used a two component model to describe a technique for measuring the lifetimes of atomic states of the projectile moving in a solid. The two-component model is structured to account for projectiles moving in the target with or without a single K-shell vacancy. Hopkins²⁶ has reported the use of the two-component model to describe the vacancy fractions of Cl ions moving in thin carbon foils prior to striking a thin Cu layer on the carbon targets. Gray et al.²⁷ have reported

results from the present work in which an extension of the two-component model was made to describe the target thickness dependence observed in target x-ray production for Cl ions incident on thin solid Cu targets. Similarly Groenveld et al.²⁸ have studied a two-component model in connection with both projectile and target x-ray production for 10 MeV projectiles on thin Al targets.

The work presented here establishes for the first time that there exist effects associated with the thickness of the solid target when heavy ions are used to excite target K-shell x rays which have not been previously considered. The following study was undertaken to assess the magnitude of such effects as a function of Z_1/Z_2 and projectile velocity, which bring additional dimensions into the considerations of inner shell ionization by heavy ions having both experimental and theoretical importance. The goals of this work were (1) to extend the considerations of projectile vacancy production and quenching processes to include the existence of the double K-vacancy state in the projectile moving in the target (three-component model) and (2) to provide a systematic study of the production of target K x rays for incident heavy ions having charge states less than or equal to Z_1 as a basis for evaluating the theory.

CHAPTER II

EXPERIMENTAL PROCEDURE AND ANALYSIS

Measurements of Cu K x-ray production cross sections were made for incident F, Al, Si, S, and Cl ion on a variety of thin solid Cu targets. Targets ranging in thickness from 2 to $183 \mu\text{g}/\text{cm}^2$ were prepared by vacuum evaporation of Cu onto transmission-mounted C backings. The C backings were typically $40 \mu\text{g}/\text{cm}^2$ thick. In addition, a thin layer of Ag approximately $50 \mu\text{g}/\text{cm}^2$ thick was evaporated on the back side of each target to allow for normalization to Rutherford scatterings. The element, Ag, was chosen because of its high Coulomb barrier and there are no interferences in the target x-ray spectrum for Cu. This step was required by the deviations from Rutherford scattering of F on Cu observed in earlier work where the projectile energy had approached the Coulomb barrier of Cu. The ratio of Cu K x-rays to scattered F projectiles exhibited sharp oscillatory behavior as a function of target thickness due to statistical fluctuations (Ericson fluctuations) in the nuclear scattering channel. The Ag layer also allowed for the reduction in counting time normally required by the thinner Cu targets. The Cu thickness of each target was determined by using 3 MeV H^+ beam to measure the $\text{Cu}(p,p)\text{Cu}$ elastic scattering yield at a laboratory angle

of 45 degrees. The ratio, R , of the relative target thickness of Ag to that of Cu was determined in a similar manner. The uncertainty associated with the measured target thicknesses was less than or equal to 5 per cent.

Beams of F, Al, Si, S, and Cl were obtained from the model EN tandem Van de Graaff accelerator at Kansas State University. The Cu K x rays were detected by a KEVEX Si(Li) x-ray detector located outside the vacuum system at a laboratory angle of 90 degrees with respect to the beam axis. The resolution of the x-ray detector was ~ 180 eV at 5.9 keV. The x rays produced by the target reached the $30 \text{ mm}^2 \times 3 \text{ mm}$ active detector volume of the x-ray detector by passing through a 0.127-mm Mylar window in the vacuum system, a 0.381-mm Mylar absorber used to reduce the count rate associated with lower energy x rays from the projectile, and a 0.025 mm Be window on the detector. A standard electronic arrangement consisting of a bias supply, preamplifier, amplifier, analog-to-digital converter, and multi-channel analyzer was used. The absolute x-ray detector system efficiency, which includes the solid angle, the absorption of x rays, and the efficiency of the Si(Li) detector, was determined experimentally using x rays from calibrated sources as previously described by Gehrke and Lokken.²⁹ Using this technique the detector efficiency at the average Cu K x-ray energy was determined to be 2.5×10^{-4} .

The scattered ions were detected by a silicon surface barrier detector placed at a laboratory angle of 30 degrees

with respect to the beam axis. The detector, which was located inside the vacuum system, was preceded by a 4.76 mm diameter collimator. A similar electronic arrangement to that used for x-ray detection was used. The solid angle subtended by the detector with respect to the beam spot, Ω , was measured using a calibrated ^{241}Am source. The solid angle was determined to be 2.2×10^{-3} sr. using this method.

A range of pure charge states for 5^+ to 9^+ F ions, 7^+ to 13^+ Al ions, 8^+ to 14^+ Si ions, 8^+ to 16^+ S ions, and 9^+ to 16^+ Cl ions was used in the measurements. The higher charge states were obtained by passing the magnetically analyzed beam through a carbon post stripping foil and then selecting the appropriate charge state with further magnetic analysis. The ratio of the number of target K x rays, Y_X , to the number projectiles scattered by Ag, Y_{Ag} , was then measured simultaneously for each target thickness and charge state. A greater variety of target thicknesses was obtained by positioning each target at 20 degrees, 30 degrees, and 40 degrees with respect to the beam axis and recording x-ray and particle yields for each angle. The x-ray yield was determined by summing the number of counts in the $\bar{K}_\alpha$ and $\bar{K}_\beta$ peaks of the x-ray spectrum and subtracting a linear background. While for the scattered particles, the yield was determined by summing the number of counts in the Rutherford scattering peak of Ag and subtracting a linear

background. Both these sums were calculated by programs available within the computer-based multi-channel analyzers. In addition, counting rates were kept low in both detector systems so that no dead time corrections were necessary in the analysis.

Using the x-ray and particle yields, an absolute Cu K-shell x-ray production cross section was calculated for each target thickness using the formula shown in Appendix B. Since the scattering monitored was that of the projectile off Ag and not Cu, the number of scattered particles, Y_p , was taken as

$$Y_p = Y_{Ag}/R = Y_{Cu} \quad .$$

Thus the target x-ray production cross section becomes

$$\sigma_x = - \frac{\Omega}{\epsilon} \frac{d\sigma}{d\Omega} \frac{Y_x}{Y_{Ag}} R \quad .$$

The statistical error associated with each experimental point was less than 10 per cent and typically less than 5 per cent. The standard deviation of each measured cross section was primarily due to the statistical error in the x-ray and particle yields and the error in the efficiency of the x-ray detector, which was 10 per cent at 8.2 keV. Thus the deviation of each experimental cross section was at most 15 per cent and typically less than 10 per cent.

CHAPTER III

THEORY

A proper understanding of target (and projectile) x-ray production cross sections for heavy ions moving in dense media relies on a model which takes into account the K-vacancy states of the projectile as it moves through the medium. It has been shown in a limited number of cases that projectiles with K vacancies have a substantially different effect on target K-shell ionization cross sections in comparison to those projectiles with no K vacancies. Generally the target cross sections show a relatively large increase in magnitude for hydrogen-like projectiles. This feature of target K-shell ionization by heavy ions suggests that contributions to target x-ray production associated with fractions of the projectile having one or more K-shell vacancies should be included in models which describe the target x-ray production. Such an approach represents a distinct departure from considerations which are the basis of previous measurements and analyses.¹³⁻¹⁷

Two-Component Model

Previous work by Groeneveld et al.²⁸ presented the development of a two-component model which described projectiles moving in a solid target with and/or without a K

vacancy. Results by Gray et al.²⁷ report a similar approach to describe variations in target K x-ray production with target thickness for Cl ions moving in thin solid Cu targets. The basis for the two-component model rests on the concept that the fraction of projectiles with no K-shell vacancy, Y_0 , and the fraction with one K-shell vacancy, Y_1 , are related in such a manner that $Y_0 = 1 - Y_1$. Changes in the relative fractions will then be reflected in the target x-ray production as a function of target thickness. The change of these fractions with the distance, x , which the projectile has traveled in the target has been given²⁷ by the following rate equation

$$\frac{dY_1}{dx} = \sigma_{01} Y_0 - \sigma_{10} Y_1 ,$$

where σ_{if} is the total charge-changing cross section, with i representing the number of initial K-shell vacancies in the projectile and f representing the final number of K-shell vacancies in the projectile. The cross section, σ_{01} , is assumed to be a sum of the cross section for capture into the K shell of the projectile and the quenching cross section due to the decay of the K-shell vacancy in the projectile. Such a quenching cross section as that due to decay can be written as

$$\sigma_\tau = (n\tau v)^{-1} ,$$

where n is the number of projectiles per cm^3 , τ is the lifetime of the excited state in seconds, and v is the projectile

velocity in cm per second. Integration of the rate equation then yields

$$Y_1 = \frac{\sigma_{01}}{\sigma} (1 - e^{-\sigma x}) + A e^{-\sigma x} ,$$

where $\sigma = \sigma_{01} + \sigma_{10}$, and A is the fraction of incident projectiles with a K vacancy. Since an enhancement in the target x-ray yield is observed for projectiles with a K-shell vacancy compared to projectiles without a K-shell vacancy, it can be assumed that $\sigma_{K1} = \alpha \sigma_{K0}$, where σ_{K1} and σ_{K0} are the target K x-ray production cross sections for projectiles with and without a K-shell vacancy respectively. Using this assumption along with a weighted average target K x-ray cross section, $\overline{\sigma_{KX}}$, yields

$$\overline{\sigma_{KX}} = \frac{\sigma_{K0}}{T} \int_0^T \{1 + (\alpha - 1) Y_1\} dx$$

and thus

$$\overline{\sigma_{KX}} = \sigma_{K0} \left\{ 1 + (\alpha - 1) \frac{\sigma_{01}}{\sigma} - \frac{\alpha - 1}{T} \left(\frac{\sigma_{01}}{\sigma} - A \right) (1 - e^{-\sigma T}) \right\} .$$

It is noted for an enhancement of $\alpha = 1$ that the averaged target cross section becomes independent of the target thickness, and hence $\overline{\sigma_{KX}}$ is the target K-shell x-ray production cross section. However for $\alpha > 1$, the measured target x-ray yield will depend on the target thickness to varying degrees depending upon the boundary conditions, the ratio of σ_{01}/σ for the projectile, and the strength of the enhancement, α . In the case where the target x-ray yield is measured for projectiles with no K-shell vacancies, the appropriate

target cross section for comparison to theory is σ_{K0} .

For initial studies of Cl^{q+} ions incident on Cu at 1.71 MeV/amu where only ions of $q \leq Z_1 - 1$ were available,²⁷ the two-component model provided an adequate description of the target x-ray yields. However, for ions lighter than Cl where $q \leq Z_1$, the two-component model breaks down. The two-component description of $\overline{\sigma_{KX}}$ contains only one exponential term which is raised to a negative power, and hence it requires that the target x-ray production cross section either decrease or remain constant as a function of target thickness for incident ions with $q = Z_1 - 1$. This is not always the case since it is possible in some cases for $\overline{\sigma_{KX}}$ to increase with increasing target thickness.

Three-Component Model

In order to explain this behavior, it is necessary to include the possibility of double K-shell vacancies in the projectile. This extension of the two-component model for charge-changing collisions was summarized by Allison.²⁴ In the three-component model the rate equations describing the projectile vacancies may be written as follows:

$$\frac{dY_2}{dx} = \sigma_{02}Y_0 + \sigma_{12}Y_1 - (\sigma_{20} + \sigma_{21})Y_2$$

$$\frac{dY_1}{dx} = \sigma_{01}Y_0 - (\sigma_{12} + \sigma_{10})Y_1 + \sigma_{21}Y_2$$

$$1 = Y_0 + Y_1 + Y_2 \quad ,$$

where the different projectile cross sections are

characterized in Figure 1.

Using the initial number of projectile K vacancies as boundary conditions to solve these rate equations yield vacancy fractions of the form

$$Y_j = F_{j\infty} + P(i,j)e^{f(\sigma_{if})T} + N(i,j)e^{-f'(\sigma_{if})T},$$

where $F_{j\infty}$ is the equilibrium fraction of ions with j K-shell vacancies, $P(i,j)$ and $N(i,j)$ are functions of the boundary conditions with i equal to the number of initial K-shell vacancies in the projectile and j equal to the number of K-shell vacancies under consideration, and $f(\sigma_{if})$ and $f'(\sigma_{if})$ are functions of the projectile cross sections. The solutions of the rate equations are obtained by diagonalizing the coefficient matrix of Y_i ($i = 0,1,2$) and assuming exponential forms for the solutions.³⁰ The expressions for $F_{j\infty}$, $P(i,j)$, $N(i,j)$, $f(\sigma_{if})$, and $f'(\sigma_{if})$ are presented in Appendix C.

The target x-ray production cross section may be written in terms of the contributions from the individual projectile K-vacancy fractions weighted over the target thickness. However, now there exists not only the single K-shell vacancy enhancement, but also a double K-shell vacancy enhancement, β . Thus

$$\overline{\sigma_{KX}} = \frac{\sigma_{K0}}{T} \int_0^T \{1 + (\alpha - 1)Y_1 + (\beta - 1)Y_2\} dx,$$

where $\sigma_{K1} = \alpha \sigma_{K0}$ and $\sigma_{K2} = \beta \sigma_{K0}$. Note that $\overline{\sigma_{KX}} = \sigma_{K0}$ only for enhancements of $\alpha = 1$ and $\beta = 1$.

Figure 1. Characteristics of Projectile Cross Sections

The general solution of this integral may be written as:

$$\begin{aligned} \overline{\sigma}_{KX} = & \sigma_{K0} \{ 1 + (\alpha-1) \{ F_{1\infty} + \frac{P(i,1)}{f(\sigma_{if})^T} (e^{f(\sigma_{if})^T} - 1) \\ & - \frac{N(i,1)}{f'(\sigma_{if})^T} (e^{-f'(\sigma_{if})^T} - 1) \} + (\beta-1) \{ F_{2\infty} + \frac{P(i,2)}{f(\sigma_{if})^T} \\ & \times (e^{f(\sigma_{if})^T} - 1) - \frac{N(i,2)}{f'(\sigma_{if})^T} (e^{-f'(\sigma_{if})^T} - 1) \} \} . \end{aligned}$$

The character of the solutions when $\sigma_{if} \approx \sigma_{fi}$ is illustrated in Figure 2. In general, the target x-ray production cross section for ions with charge $q \leq Z_1 - 2$ increases toward a saturation value given by

$$\overline{\sigma}_{KX} = \sigma_{K0} \{ 1 + (\alpha-1)F_{1\infty} + (\beta-1)F_{2\infty} \} .$$

For ions with charge $q = Z_1 - 1$ and $q = Z_1$, $\overline{\sigma}_{KX}$ decreases exponentially with target thickness toward the saturation value. Since the solutions for the three-component model are sums of exponentials, the general character of the solutions strongly depends upon the relative strengths of the vacancy production and quenching interactions for the projectile. Hence the behavior of the target x-ray production cross section will reflect these relative strengths and the coupling of those vacancies to the target K shell. It should be noted that the saturation value of the cross section is representative of a target sufficiently thick to allow the K-vacancy fractions to equilibrate, thus removing the target thickness dependence from the equation for $\overline{\sigma}_{KX}$.

Figure 2. Characteristics of Three-Component Model

N-Component Model

An extension of the three-component model to a n-component model, where n is now the number of charge states that contribute to the process in question, is straightforward. The technique is based on the solution of n rate equations such that $\sum Y_n = 1$. Once each individual component, Y_n , has been found, $\overline{\sigma_{KX}}$ can be determined by averaging the weighted components over the target thickness such that

$$\overline{\sigma_{KX}} = \sigma_{K0} \int_0^T \{1 + \sum (a_n - 1) Y_n\} dx \quad .$$

While the technique is straightforward, the complexity of the algebra plus the success of the three-component model makes such an extension unwarranted at this time.

CHAPTER IV

EXPERIMENTAL RESULTS AND COMPARISON WITH THEORY

$\overline{\sigma}_{\text{KX}}$ Versus Z_1

An experimental check of the two-component model was performed using 1.71 MeV/amu Cl^{q+} incident on thin solid Cu targets. For this case q was less than Z_1 . Shown in Figure 3 is the ratio of Cu K x rays per scattered projectile, Y_X/Y_P , for Cl charge states from 9+ to 16+. The data remains essentially constant for charge states from 9+ to 14+. Then at 15+ the data show an increase of approximately 8 per cent, which is believed to be due to a small fraction of helium-like metastable projectiles possessing a K-shell vacancy. Finally there is a large enhancement in Y_X/Y_P for projectiles with one K vacancy, Cl^{16+} . It should also be noted that this enhancement is observed in all three Cu target thicknesses shown in Figure 3. This includes the 92.1 $\mu\text{g}/\text{cm}^2$ target, which is well past what was previously considered to be the equilibrium target thickness.

The averaged target x-ray production cross section, $\overline{\sigma}_{\text{KX}}$, is shown in Figure 4 as a function of target thickness for 1.71 MeV/amu Cl on Cu. The solid lines represent the best fit from the two-component model, where data from projectiles with ($A=1$) and without ($A=0$) K vacancies were

Figure 3. Y_X/Y_P Versus Charge State of Cl^{q+}

Figure 4. $\overline{\sigma_{KX}}$ of Cu for Cl^{q+} Bombardment

fit simultaneously. The general trends of $\overline{\sigma}_{KX}$ are easily observed, an exponential increase for projectiles with no K vacancy and an exponential decrease for projectiles with a K vacancy. The fitted value of the enhancement of σ_{K1} over σ_{K0} is approximately 8. Shown also in Figure 4 is the saturation value of $\overline{\sigma}_{KX}$ which is given as the dashed line.

Studies of the three-component model were performed using F, Al, Si, and S ions at 1.71 MeV/amu on Cu targets. In addition the three-component model was used to fit the Cl data for a consistency check. The three-component model reproduced within the fitting error the fit of the two-component model.

Figure 5 depicts the data for F on Cu with the best fits from the three-component model. These calculations have been performed using a least-squares method (See Appendix D) which fits all data simultaneously with a single set of parameters, i.e., projectile cross sections, enhancement factors, and σ_{K0} . The general character of the data gives a restricted range of values for the enhancement factors, α and β , and the target K-shell x-ray cross section for a vanishingly thin target, σ_{K0} . Initial estimates of σ_{if} were made and the least squares fit performed. For hydrogen-like F ions at 1.71 MeV/amu incident on Cu, it is clear that the target x-ray cross section does not decrease with thickness. Just such a case illustrates the need for the third component.

Figure 5. $\overline{\sigma}_{KX}$ of Cu for F^{q+} Bombardment

The measurements of $\overline{\sigma_{KX}}$ for Al, Si, and S ions on Cu are given in Figure 6 along with the model fits to the data. The data for the systems studied are given in Table I. In contrast to the F data, the decrease of the target x-ray cross section with thickness for $q = Z_1 - 1$ illustrates the change in relative K-vacancy populations for the heavier projectiles. In addition, the increase in the enhancement factors, α and β , with increasing atomic number of the projectiles at a fixed value of 1.71 MeV/amu is easily observed.

By the use of the vacancy production and quenching cross sections, the K-shell vacancy fractions for the projectiles are calculated as a function of target thickness. The results of these calculations are given in Table II. In the case of F on Cu the fractions are given in Figure 7. It is seen that the Y_2 fraction is dominant. The strong vacancy and quenching cross sections σ_{12} and σ_{10} deplete the Y_1 fraction to allow the buildup of the Y_2 and Y_0 fractions within the target. As the atomic number of the projectile is increased the Y_2 fraction decreases while the Y_0 fraction increases at a given depth within the Cu target. This effect, due to the dominance of the projectile quenching cross sections, is easily seen by comparing the F K-vacancy fractions in Figure 7 to the S K-vacancy fractions in Figure 8. The equilibration values of Y_{i0} , Y_{i1} , and Y_{i2} are listed in Table III for each projectile species. These values, which represent the equilibration fraction of the beam with zero,

Figure 6. σ_{KX} of Cu for Al^{q+} , Si^{q+} , and S^{q+} Bombardment

TABLE I

VALUES OF $\overline{\sigma}_{\text{KX}}$ FOR DIFFERENT PROJECTILE CHARGE
STATES INCIDENT ON Cu AT 1.71 MeV/amu

Projectile	Target Thickness ($\mu\text{g}/\text{cm}^2$)	Cross Section (barns)		
		for $q < Z_1 - 1$	for $q = Z_1 - 1$	for $q = Z_1$
F^{q+} ($Z_1=9$)	3.1	440	524	655
	3.8	491	529	679
	6.0	517	584	727
	7.4	514	583	738
	8.6	511	568	688
	9.3	527	596	689
	10.5	532	611	686
	12.8	522	588	668
	13.9	552	619	694
	15.7	543	612	684
	18.9	548	622	652
	20.6	547	625	666
	23.2	558	648	620
	28.9	557	570	638
	92.1	584	598	591

Projectile	Target Thickness ($\mu\text{g}/\text{cm}^2$)	Cross Section (barns)		
		for $q < Z_1 - 1$	for $q = Z_1 - 1$	for $q = Z_1$
Al^{q+}	3.1	683	11490	2257
$(Z_1=13)$	3.8	671	1517	2240
	6.0	716	1437	
	7.4	689	1443	2195
	8.6	778	1532	2322
	10.5	783	1488	
	12.8	759	1410	2219
	15.7	772	1379	2059
	18.9	785	1365	
	20.6	785	1390	
	23.2	881	1300	
	28.3	883	1256	
	32.0	904	1263	
	44.7	836	1182	1535
	48.5	872	1147	
	54.8	885	1142	
	69.3	852	1060	1300
	75.2	895	1053	
	85.0	825	1030	1396
Si^{q+}	3.1	815	2095	
$(Z_1=14)$	3.8	765	2199	

Projectile	Target Thickness ($\mu\text{g}/\text{cm}^2$)	Cross Section (barns)		
		for $q < Z_1 - 1$	for $q = Z_1 - 1$	for $q = Z_1$
Si^{q+}	6.0	813	2243	
	7.4	811	2040	
	8.6	913	2233	4221
	10.5	886	2015	
	12.8	861	1975	
	15.7	907	2002	
	18.9	1001	1925	
	20.6	1001	1891	2830
	23.2	991	1757	
	26.1	964	1898	
	28.3	980	1774	
	32.0	1003	1739	
	44.7	978	1699	
	48.5	987	1693	2204
	54.8	1022	1605	
	69.3	1041	1525	2011
	75.2	1033	1449	
	85.0	1045	1479	1879
S^{q+}	3.1	1008		
$(Z_1=16)$	3.3	1006		
	3.8	911	4787	

Projectile	Target Thickness ($\mu\text{g}/\text{cm}^2$)	Cross Section (barns)		
		for $q < Z_1 - 1$	for $q = Z_1 - 1$	for $q = Z_1$
S^{q+}	6.0	992		
	6.5	1068	5156	
	7.4	1064	5001	
	8.6	1099	5195	
	9.3	1185	5487	10274
	10.5	1218		
	12.8	1195	5370	
	13.9	1193	5468	
	15.7	1222	5020	9067
	18.9	1383	4845	
	20.6	1440		
	23.2	1440	4495	
	44.7	1506	4436	8250
	54.8	1652	4145	7355
	69.3	1605	3950	
	75.1	1613		
	79.5		3853	
	85.0	1662	3697	5448
Cl^{q+}	3.02	1172		
(Z ₁ =17)	4.08		8412	
	4.27	1232		

Projectile	Target Thickness ($\mu\text{g}/\text{cm}^2$)	Cross Section (barns)		
		for $q < Z_1 - 1$	for $q = Z_1 - 1$	for $q = Z_1$
Cl^{q+}	7.3		9711	
	12.0		9853	
	13.7	1381		
	15.2	1402		
	20.8	1495	8203	
	27.9	1603		
	28.9		7857	
	38.0	1642		
	44.1		7416	
	51.9	1817		
	58.5	1814		
	59.8		7659	
	65.2	1903		
	67.4	1911		
	75.2	1976	6949	
	79.9	2000		
	92.1	2058	6137	
	113.0		5562	
	176.0	2362	4610	

TABLE II

K-VACANCY FRACTIONS FOR DIFFERENT PROJECTILE
CHARGE STATES INCIDENT ON Cu AT 1.71 MeV/amu

Projec- tile	Target Thickness ($\mu\text{g}/\text{cm}^2$)	K-Vacancy Fraction								
		Y_{00}	Y_{01}	Y_{02}	Y_{10}	Y_{11}	Y_{12}	Y_{20}	Y_{21}	Y_{22}
F^{q+} ($Z_1=9$)	1.1	0.85	0.12	0.03	0.30	0.41	0.29	0.04	0.06	0.88
	5.3	0.59	0.16	0.25	0.42	0.15	0.43	0.21	0.13	0.66
	10.6	0.47	0.15	0.38	0.40	0.14	0.46	0.32	0.13	0.55
	15.8	0.42	0.14	0.44	0.39	0.14	0.47	0.36	0.14	0.50
	20.1	0.41	0.14	0.45	0.39	0.14	0.47	0.38	0.14	0.48
	30.6	0.39	0.14	0.47	0.39	0.14	0.47	0.39	0.14	0.47
	40.1	0.39	0.14	0.47	0.39	0.14	0.47	0.39	0.14	0.47
Al^{q+} ($Z_1=13$)	1.2	0.98	0.02	0.00	0.01	0.98	0.01	0.00	0.01	0.99
	5.4	0.93	0.05	0.02	0.36	0.46	0.18	0.14	0.21	0.65
	10.7	0.88	0.08	0.04	0.52	0.27	0.21	0.29	0.24	0.47
	14.9	0.86	0.09	0.05	0.59	0.20	0.21	0.39	0.23	0.38
	20.2	0.83	0.10	0.07	0.65	0.17	0.18	0.50	0.20	0.30
	30.7	0.81	0.11	0.08	0.71	0.14	0.15	0.63	0.16	0.21
	40.2	0.79	0.11	0.10	0.74	0.13	0.13	0.69	0.14	0.17
	50.8	0.78	0.11	0.11	0.76	0.12	0.12	0.73	0.13	0.14
	60.3	0.78	0.11	0.11	0.76	0.12	0.12	0.75	0.12	0.13

Projec- tile	Target Thickness ($\mu\text{g}/\text{cm}^2$)	K-Vacancy Fraction								
		Y_{00}	Y_{01}	Y_{02}	Y_{10}	Y_{11}	Y_{12}	Y_{20}	Y_{21}	Y_{22}
Al^{q+}	70.8	0.78	0.11	0.11	0.77	0.12	0.11	0.76	0.12	0.12
	80.3	0.77	0.12	0.11	0.77	0.12	0.11	0.77	0.12	0.11
	90.9	0.77	0.12	0.11	0.77	0.12	0.11	0.77	0.12	0.11
Si^{q+}	1.1	1.00	0.00	0.00	0.01	0.99	0.00	0.00	0.01	0.99
$(Z_1=14)$	5.4	0.95	0.04	0.01	0.35	0.50	0.15	0.13	0.19	0.68
	10.7	0.91	0.06	0.03	0.52	0.30	0.18	0.28	0.23	0.49
	14.9	0.89	0.07	0.04	0.61	0.22	0.17	0.38	0.23	0.39
	20.2	0.87	0.07	0.06	0.67	0.17	0.16	0.49	0.20	0.31
	30.7	0.85	0.08	0.07	0.75	0.13	0.12	0.64	0.16	0.20
	40.2	0.84	0.09	0.07	0.78	0.11	0.11	0.72	0.13	0.15
	50.8	0.83	0.09	0.08	0.80	0.10	0.10	0.77	0.12	0.11
	60.3	0.83	0.09	0.08	0.81	0.10	0.09	0.79	0.11	0.10
	70.8	0.83	0.09	0.08	0.82	0.10	0.08	0.81	0.10	0.09
	80.3	0.83	0.09	0.08	0.82	0.10	0.08	0.81	0.10	0.09
	90.9	0.83	0.09	0.08	0.83	0.09	0.08	0.82	0.10	0.08
S^{q+}	1.1	1.00	0.00	0.00	0.01	0.99	0.00	0.00	0.00	1.00
$(Z_1=16)$	5.4	0.97	0.02	0.01	0.24	0.60	0.16	0.09	0.07	0.84
	10.7	0.95	0.03	0.02	0.39	0.38	0.23	0.18	0.10	0.72
	14.9	0.94	0.04	0.02	0.47	0.27	0.26	0.25	0.11	0.64
	20.2	0.93	0.04	0.03	0.55	0.19	0.26	0.33	0.11	0.56

Projec- tile	Target Thickness ($\mu\text{g}/\text{cm}^2$)	K-Vacancy Fraction								
		Y_{00}	Y_{01}	Y_{02}	Y_{10}	Y_{11}	Y_{12}	Y_{20}	Y_{21}	Y_{22}
S^{q+}	30.7	0.91	0.05	0.04	0.64	0.11	0.25	0.46	0.11	0.43
	40.2	0.89	0.05	0.06	0.70	0.09	0.21	0.55	0.10	0.34
	50.8	0.88	0.05	0.07	0.74	0.07	0.19	0.62	0.09	0.29
	60.3	0.87	0.05	0.08	0.77	0.07	0.16	0.68	0.08	0.24
	70.8	0.87	0.05	0.08	0.79	0.07	0.14	0.72	0.07	0.21
	80.3	0.86	0.05	0.08	0.80	0.06	0.14	0.75	0.07	0.18
	90.9	0.86	0.05	0.08	0.81	0.06	0.13	0.78	0.07	0.15
	104.6	0.86	0.05	0.08	0.82	0.06	0.12	0.80	0.06	0.14

Figure 7. K-Vacancy Fractions of F^{q+} in Cu

Figure 8. K-Vacancy Fractions of S^{q+} in Cu

TABLE III

VALUES OF EQUILIBRATION FRACTION, $F_{j\infty}$, FOR 1.71 MeV/amu
IONS INCIDENT ON Cu TARGETS

$Z_{1\infty}$	$F_{0\infty}$	$F_{1\infty}$	$F_{2\infty}$
9	0.39	0.14	0.47
13	0.77	0.12	0.11
14	0.83	0.09	0.08
16	0.85	0.06	0.09

one, and two K vacancies respectively, are used to calculate the saturation value of $\overline{\sigma}_{\text{KX}}$. The saturation values of $\overline{\sigma}_{\text{KX}}$ along with the approximate target thickness at which they occur are shown in Table IV.

The systematics of the parameters in the expression for $\overline{\sigma}_{\text{KX}}$ are shown in Figure 9.. Comparison to estimates from other sources, where available, are shown. Calculations for the projectile quenching cross sections σ_{10} and σ_{21} have been performed using the Brinkman-Kramers formulation of charge exchange as given by Nikolaev.³¹ A scaling factor of 1/9 has been introduced to give the estimates shown for these two cross sections in Figure 9a. The scale factor of 1/9 is in agreement with earlier work by Hopkins²⁶ for Cl on Cu. The values of σ_{10} and σ_{21} obtained from the fits to the data for $\overline{\sigma}_{\text{KX}}$ follow the general trends given by the scaled Brinkman-Kramers estimates. It is important to point out that while the projectile quenching cross section is a sum of the charge exchange to the K shell and the decay to the K shell, the cross section is being compared to calculations which consider only the charge exchange part. This is justifiable when comparing trends since the decay cross section is small compared to the charge exchange cross section for all the projectiles studied except Cl. The double quenching cross section, σ_{20} , as obtained from the fits is essentially independent of Z_1 , but it should be noted that since double quenching is much less than single quenching,

TABLE IV

TARGET X-RAY CROSS SECTION AT SATURATION, $\overline{\sigma}_{\text{KX}}^{\text{SAT}}$,
AND SATURATION THICKNESS, T^{SAT}

Z_1	$\overline{\sigma}_{\text{KX}}^{\text{SAT}}$ (b)	T^{SAT} ($\mu\text{g}/\text{cm}^2$)
9 (F)	604	≈ 40
13 (Al)	983	≈ 100
14 (Si)	1197	≈ 200
16 (S)	2202	≈ 500
17 (Cl)	2730	≈ 1000

Figure 9. Systematics Versus Z_1

the fits are relatively insensitive to the double quenching cross section. In Figure 9b the projectile vacancy production cross sections are given. The cross sections σ_{01} , σ_{12} , and σ_{02} are interactions which create one and two K-shell vacancies in the projectiles and are thought to contain both ionization and excitation processes. The short-dashed lines in Figure 9b are eye guides. There appears at present to exist no reliable estimates or data upon which a comparison of these cross sections can be based. It is noted that the σ_{12} cross section is larger than σ_{01} with the ratio of these two cross sections increasing by a factor of ~ 5 in going from F to S on Cu. Because of binding energy considerations it would be expected that $\sigma_{12} < \sigma_{01}$ if the dominant mechanism was a direct Coulomb interaction. On the other hand if the dominant interaction was a vacancy transfer type of mechanism, then the increased binding energy of the Y_1 system over the Y_0 system could favor the enhancement of the σ_{12} cross section. The fits to the data require $\sigma_{12} > \sigma_{01}$ consistently, and certainly this is facet of the present description of the target x-ray production process which requires additional investigation. Calculations in which $\sigma_{02} = 0$ lead to a larger divergence in σ_{12} and σ_{01} with $\sigma_{12} \approx 20 \sigma_{01}$ for S ions on Cu. The double vacancy cross section, σ_{02} , is generally down in strength by an order of magnitude or more as expected from measurement of K-shell hypersatellite production, which is generally < 10

per cent of the satellite strength for elements in the Z_1 range of the projectiles used in the present work.³²

The experimental values of σ_{K0} are given in Figure 9c for the incident ions F, Al, Si, S, and Cl at 1.71 MeV/amu. Plane wave Born approximation (PWBA) calculations for σ_{K0} are shown in the figure. The PWBA calculations overestimate the cross sections by an order of magnitude. This trend is in agreement with the systematics from earlier work¹⁶ for lighter ions on elements in the range of Cu. In order to obtain an estimate of σ_{K0} it is assumed that there are two mechanisms for creating K vacancies in the target; direct Coulomb ionization and charge exchange from the 1s shell of the target to projectile states having $n \geq 2$. Brinkman-Kramers calculations for the charge exchange component were scaled by a factor of 1/9 and multiplied by the atomic value of ω_K for Cu to give the cross section σ_{BK} . Calculations for the direct Coulomb contribution were taken from Brandt and Lapicki³³ for the PWBABC. As has been shown earlier^{13,16} the binding energy correction causes a large reduction in the calculated cross sections. The value of σ_{K0} was then taken to be

$$\sigma_{K0} = \sigma_{PWBABC} + \sigma_{BK} \quad .$$

The individual contributions for σ_{BK} and σ_{PWBABC} are shown in Figure 9c. The estimates for σ_{K0} as described above give qualitative agreement with the experimental data. This agreement can be seen over a wider range of projectile

atomic numbers. Figure 10 shows σ_{K0} for H up to Cl on Cu all at 1.71 MeV/amu. Also shown are the saturation value of $\overline{\sigma_{KX}}$, $\overline{\sigma_{KX}^{SAT}}$, and the target x-ray production cross section for ions with two K vacancies incident on a vanishingly thin Cu target, σ_{K2} . As can be easily observed there appears to be no target thickness dependence for ions lighter than C or O on Cu, but for ions heavier than these there exists a noticeable discrepancy between σ_{K0} , $\overline{\sigma_{KX}^{SAT}}$, and σ_{K2} . Figure 11 shows the same data with the addition of σ_{PWBABC} , σ_{BK} , and $\sigma_{PWBABC} + \sigma_{BK}$ for comparison purposes. Also shown is the product of β and $\sigma_{PWBABC} + \sigma_{BK}$ for comparison to σ_{K2} .

The parameters α and β obtained from the data are given in Figure 9d. The calculated values of α and β are based upon the following equations

$$\alpha = \frac{\sigma_{K0} + w\omega\pi R^2}{\sigma_{K0}}$$

and

$$\beta = \frac{\sigma_{K0} + 2w'\omega\pi R^2}{\sigma_{K0}},$$

where ω is the neutral atom fluorescence yield for Cu. Estimates³⁴ of the effects of multiple ionization on ω for Cu show that the change in ω should be ~ 15 per cent. Hydrogen-like and helium-like binding energies³⁵ were used in the calculation of w' and w , the Meyerhof vacancy transfer probabilities,¹⁸ for the $q = Z_1$ and $q = Z_1 - 1$ charge states of the incident ion, where

Figure 10. σ_{K0} , $\frac{\sigma_{KX}}{\sigma_{KX}^{SAT}}$, and σ_{K2} Versus Z_1

Figure 11. Theory Versus Data of Figure 10

$$w = \frac{1}{1 + e^{2|x|}}$$

and

$$x = \frac{13.6}{v_1} \frac{I_2 - I_1}{(I_2)^{\frac{1}{2}} + (I_1)^{\frac{1}{2}}}$$

with v_1 equal to the projectile velocity in atomic units and I_1 and I_2 equal to the binding energy of the projectile and target respectively. In addition, the factor of two found in the equation for β comes from the fact that there are two vacancies available to be transferred to the target. The values of R were taken from the peaks of the dynamic coupling elements as given by Taulbjerg *et al.*³⁶ The agreement between the data and predictions of the proposed model for α and β support the hypothesis that the 1s to 1s vacancy transfer mechanism is a plausible interaction by which the x-ray production cross section is enhanced for the bare and hydrogen-like incident ions. Halpern and Law³⁷ have suggested that such enhancements are due to the addition of a charge exchange component to the direct Coulomb component of the target x-ray production cross section instead of a vacancy transfer component. While the end results are the same, there exists no quantitative way to calculate the fraction due to charge exchange, and therefore Halpern and Law's results are based purely on fits of the data to obtain this fraction.

$\overline{\sigma_{KX}}$ Versus E_1

In addition to the systematics of target thickness effects as a function of incident projectile atomic number, it is also of interest to examine such effects as a function of incident projectile energy, E_1 . Figure 12 shows the values of $\overline{\sigma_{KX}}$ for Cl^{q+} at 40, 50, and 60 MeV incident upon Cu. In each case q was less than $Z_1 - 1$ so that there were no K-shell vacancies in the incident projectile. The solid lines are eye guides since at the lower energies the hydrogen-like Cl on Cu data could not be taken. For all the projectile energies shown there exist a strong target thickness dependence, although the effect does appear to decrease with energy.

Figure 13 shows a similar trend for 1.7, 2.0, 2.2, and 2.5 MeV/amu F^{q+} on Cu. Once again q is less than $Z_1 - 1$ in all cases. In this figure the solid lines represent fits by the three-component model. As before, a strong target thickness dependence is evident in $\overline{\sigma_{KX}}$, and the effect appears to decrease with the projectile energy. The values of σ_{K0} , α , and β obtained from the three-component fits of this F on Cu data are shown in Figure 14. Also shown are several different calculated values for comparison purposes. Once again the sum of σ_{PWBABC} and σ_{BK} appears to show the general trend of σ_{K0} . It is important to note that while this sum is below the experimental values, all σ_{BK} cross sections have been scaled by a factor of 1/9. If a more qualitative approach to scaling was applied it is possible that

Figure 12. $\overline{\sigma_{\text{KX}}}$ of Cu Versus Energy of Cl^{q+}

Figure 13. $\overline{\sigma}_{KX}$ of Cu Versus Energy of F^{q+}

Figure 14. Systematics Versus E_1

such a sum would come much closer to the data. Second, the calculations for α and β based on a vacancy transfer mechanism show the trend of the experimental values as before. It can be seen that as the F^{q+} energy increases, the values for α and β decrease. While this may appear to be a contradiction to the trend observed in Figure 13, in fact, it is not. The vacancy transfer approach is centered around a quasimolecular type of theory. In such a theory, vacancy transfer is not a major factor until the incident projectile energy is high enough to allow for the overlap of target and projectile K-shell wave functions. At the same time, any significant increase in the projectile energy above this overlap energy would only serve to decrease the vacancy transfer mechanism since the higher energy would require the overlap to occur for a shorter time. This is exactly the case for the values of α and β derived from F^{q+} on Cu. For the case of $\overline{\sigma}_{KX}$ shown in Figure 13, the target cross section is that produced by projectiles with no K vacancies, and therefore the mechanisms for ionization are described by the direct Coulomb and charge exchange interactions.

CHAPTER V

CONCLUSION

In summary, the systematics of thin solid target K x-ray production for heavy ions incident on Cu have been illustrated. The dependence of the target x-ray yield on the target thickness and projectile atomic number establishes the need for a model which includes effects for K-vacancy fractions in the projectile and the coupling of those vacancies to the target K shell. The importance of inner-shell vacancy configurations in heavy ions moving in solid targets has been established for the first time by the present work. The experimental results of the present work suggest that the dominant role of such vacancy distributions is distinct from previous considerations which have only considered the effects of the charge state of the incident ion species or changes in the charge state of the projectile associated with processes such as dynamic electron screening. The models presented in the present work have been developed to account for the microscopic interactions which govern the states of the ion and target atoms through the strong coupling that can exist between the ion-solid and ion-atom systems. The three-component model which is presented can satisfy the requirements for a more definitive approach to the design and execution of experiments and the interpretation of data for

x-ray production in the case of high velocity heavy ions incident upon solid targets. The major conclusion which has been established is that the vacancy configuration, not necessarily the charge state of the incident ion, is the single most important consideration in heavy ion-solid target x-ray production studies. Clearly previous solid target x-ray production cross sections from heavy ion bombardment at high velocities which do not include the effects established in the present work may not provide an adequate basis for direct testing of either the direct Coulomb or quasimolecular theories for inner-shell ionization. The complexity of x-ray production for heavy ions incident on solids and the lack of sufficient data for projectile vacancy production and quenching processes suggest that correcting existing data derived from a single target thickness measurements would be difficult if not impossible.

The systematics of the single-vacancy production cross sections for the projectile represents an area which is in need of further investigation. It is not clear that the charge exchange cross sections which involve the removal of K-shell electrons³⁸ are directly comparable to the K-vacancy production cross section derived from the three-component model. The model is sensitive to the existence of a single- or double-vacancy state in the K shell of the projectile. No distinction is made between excitation or ionization which leads to the creation of a projectile K vacancy.

Further tests of the three-component model may provide the basis for understanding the nature of the projectile vacancy production processes in solids. In addition, a more rigorous approach to determine the proper scaling of the charge exchange cross section is necessary in order to obtain better estimates of the projectile quenching cross section and σ_{K0} . With the availability of reasonable estimates for all the projectile and target parameters, extensive testing of the three-component model could then be undertaken. With such tests over a wide range of projectile atomic numbers and projectile energies, a complete evaluation of the three-component model could then be made, and any need for its extension to handle such cases as incident metastables determined. Testing in the form of application of the three-component model to the evaluation of target L-shell x-ray production cross sections as a function of target thickness have already begun by Gray and coworkers³⁹. Additionally work by Kauffman et al.⁴⁰ and Hopkins^{41, 42} suggests that studies of the K-shell ionization process for heavy ions on solid targets using high resolution x-ray spectroscopy may lead to a better understanding of the complexities involved. Gray, Schiebel, and Richard⁴³ are presently investigating appropriate ion-target systems for such studies. The three-component model provides a sound basis for further investigations.

In the case of x-ray production for heavy ions incident

upon solid targets the comparisons of theoretical calculations for inner shell ionization should be made to experimental cross sections measured for vanishingly thin targets. The relevant target cross sections for such comparisons are σ_{K0} , σ_{K1} , and σ_{K2} for incident projectile charge states of $Z_1 - 2$, $Z_1 - 1$, and Z_1 respectively. Measurements of heavy ion target x-ray production on target having a thickness of the order $\sim 10^{-5}$ g/cm² result in cross section which can deviate significantly from the results required for comparisons to existing inner shell ionization theories. A definite advance in our collective understanding of ion-atom collisions has been achieved with the present work. It remains to be seen what effect the long term ramifications of the present work may hold for future developments in both theory and experimentation in this important area of study.

APPENDIX A

Discussed in this appendix are a few of the theories used to calculate x-ray production cross sections of targets under bombardment by charged particles. Each discussion presented here is very cursory and is meant to be only an introduction to the major points. Also each theory is presented in a form for calculation of K-shell ionization cross sections. Their use as x-ray cross sections requires that they be multiplied by the proper fluorescence yield.

PWBA

In the PWBA the differential scattering cross section is given as

$$\frac{d\sigma}{d\Omega} \propto |\langle \psi_f | V | \psi_i \rangle|^2 .$$

If the interaction is assumed to be a direct Coulombic interaction between the incident ion and the target electron, the interaction potential is given as

$$V = \frac{Z_1 e^2}{|\bar{r}_1 - \bar{r}_2|} ,$$

where $Z_1 e^2$ is the charge of the projectile, $\bar{r}_1$ is the vector from the target nucleus to the projectile, and $\bar{r}_2$ is the vector connecting the target nucleus to the atomic electron. Using a product of nonrelativistic hydrogenic wave function

and a plane wave, $e^{(i\vec{p}\cdot\vec{r}_2/\hbar)}$, as the initial and final wave function, ψ_i and ψ_f , integrating over all directions, and summing over all substates of an initially filled atomic shell, s , yields⁴⁴

$$d^2\sigma_{\epsilon S} = 8\pi Z_1^2 \left(\frac{e^2}{\hbar v}\right)^2 \frac{2dq}{q^3} F_{\epsilon S}(q)^2 d\epsilon$$

where ϵ is the amount of energy transferred to the target atom, q is proportional to the momentum transferred, and $F_{\epsilon S}(q)$ is the form factor,

$$|F_{\epsilon S}(q)| = \langle \psi_f(\vec{r}_2) | e^{i\vec{q}\cdot\vec{r}_2} | \psi_i(\vec{r}_2) \rangle.$$

Using the dimensionless parameters $w = \epsilon/(Z_s^2 R_\infty)$ and $Q = a_0^2 q^2 / Z_s^2$ where Z_s is the screened nuclear charge for the s shell of the target,⁴⁵ R_∞ is Rydberg's constant, and a_0 is the Bohr radius and integrating over w and Q gives the cross section for ionization of the K shell in terms of the reduced parameters, η and θ , as

$$\sigma_K = \frac{8\pi a_0^2 Z_1^2}{Z_K^4 \eta_K} f_K(\eta_K, \theta_K).$$

In this expression η_K , the reduced velocity parameter, is equal to $(v_1/Z_K v_0)^2$, θ_K , the reduced binding energy, is equal to U_K/E_K , and the values of the function $f_K(\eta_K, \theta_K)$ have been published in tabular form by Khandelwal et al.¹

Inherent in the PWBA are several assumptions which should be noted. These are: (1) $Z_1 e^2 / \hbar v_1 \ll 1$; (2) the interaction is assumed to be Coulombic; (3) the interaction is assumed

to be weak, $Z_1 \ll Z_2$; (4) the projectile is assumed to be a point charge; (5) no recoil effects are considered; (6) interaction with other electrons is ignored.

Several corrections have been made to the PWBA in order to relax some of the restrictions placed on it by the assumptions made earlier and to improve the agreement between theoretical and experimental cross sections. The first of these entails an increase in the electron binding energy due to the presence of the ion at the time of ionization. This correction is made by replacing θ_K with $\epsilon\theta_K$ where $\epsilon > 1$.¹⁰ The second correction entails multiplying σ_K by a factor $9E_{10}$ where $9E_{10} < 1$.¹⁰ This correction, known as the Coulomb deflection correction and associated with the ion-nucleus interaction, accounts for the deflection of the projectile from a straight path during the interaction. The last of the corrections which will be discussed here is known as the polarization effect.⁴⁶ Basically this effect is an adjustment of the electron orbit to the presence of a projectile whose velocity is high enough so that the peak in the ionization cross section occurs for an impact parameter greater than the K-shell radius. The addition of such a correction, $C(\omega)$, causes an increase in the theoretical cross section at higher energies. Thus the ionization cross section with all these corrections can be written as

$$\sigma_K = \frac{72\pi a_0^2 Z_1^2}{Z_K^4 \eta_K (9 + d\pi\epsilon q_{0K})} e^{-d\pi\epsilon q_{0K}} f_K(\eta_K, \epsilon\theta_K) C(\omega) ,$$

where d is half the distance of closest approach, and q_{0K} is the minimum momentum transferred to the K-shell electron.

BEA

In the BEA it is assumed that the dominant interaction producing the transition is a direct energy exchange between the projectile and the bound electron.² The target nucleus simply establishes the momentum distribution for the electron. Thus, the collision is viewed as one between the projectile and a free electron. Since the classical and quantum mechanical expressions for the cross section of a collision between two free charged particles are identical, a classical analysis can be used to obtain the differential cross section, $d\sigma/d\Delta E$, for exchange of energy ΔE between two charged particles. Then $d\sigma/d\Delta E$ is summed over all momentum exchanges compatible with an energy exchange of ΔE and integrated over all allowable energy exchanges. Finally it is weighted by the distribution of the electron momenta associated with the bound state.

The cross section for the removal of an electron whose binding energy is U_K and whose speed is v_2 is then given by

$$\sigma_I = \int_{U_K}^E \frac{d\sigma}{d\Delta E} d\Delta E \quad .$$

Upon averaging over the momentum distribution and summing over all electrons in the shell, N_i , σ_K becomes

$$\sigma_K(v_1) = N_i \int_0^\infty \sigma_I(v_1, v_2) f(v_2) dv_2$$

where $f(v_2)$ is the momentum distribution for the bound electrons. If hydrogenic velocity distributions are used the BEA will obey the following scaling law:⁴⁷

$$U_K^2 \sigma_K = Z_1^2 f(E/U, M_1/M_2) ,$$

such that

$$\sigma_K(v) = \frac{N_i Z_1^2 \sigma_0}{U_K^2} G_K(v) .$$

To use this equation the values of $G_K(v)$ can be found in tabular form,⁴¹ and $\sigma_0 = 6.56 \times 10^4 \text{ keV}^2\text{-b}$.

SCA

In order to apply the SCA it must be possible to describe the motion of the projectile by a wave packet small compared with the distance of closest approach.⁴⁸ Thus

$$\frac{Z_1 Z_2 e^2}{\hbar v_1} \frac{\sin(\theta/2)}{1 + \sin(\theta/2)}$$

where θ is the deflection angle of the projectile. If this requirement is met then the differential cross section for the ejection of an atomic electron with final energy E_f is from first order time dependent perturbation theory given by the expression

$$\frac{d\sigma}{dE_f} = \frac{2\pi}{\hbar^2} \int_0^\infty b \, db \left| \int_{-\infty}^\infty e^{i\omega t} \langle \psi_f | V | \psi_i \rangle dt \right|^2 ,$$

where b is the impact parameter and $\omega = \Delta E/\hbar$. For a Coulomb potential and a straight projectile path in the x - z plane, this equation becomes

$$\frac{d\sigma}{dE_f} = \frac{2Z_1^2 M_1 e^4}{E_1 \hbar^2} \left| \int d\tau \psi_i \psi_f^* e^{iq_0 Z} K_0(q_0 \rho) \right|^2, \quad ,$$

where q_0 is the minimum momentum transferred, $\rho^2 = (x-b)^2 + y^2$, and $K_0(q_0 \rho)$ is a modified Bessel function of the third kind and of zeroth order. For adiabatic collisions, the K-shell cross section is given as

$$\frac{d\sigma_K}{dE_f} = \frac{2^{15} \pi m_e^7 e^{16} Z_1^2 Z_2^6}{5 \hbar^6 (U_K + E_f)^{10}} \left(\frac{E_1}{M_1} \right)^4$$

if $q_0 \gg 1/a_0$ and $q_0 \gg k$, where $\hbar k$ is the momentum of the ejected electron. The correction due to a hyperbolic path for the projectile can be expressed as

$$\frac{d\sigma_K}{dE_f} = e^{-\pi \xi} \left(\frac{d\sigma_K}{dE_f} \right)_{\text{straight}}$$

with $\xi = Z_1 Z_2 e^2 q_0 / 2E_1$.

Molecular Orbital Promotion (MO)

In the MO approach, a K-shell vacancy may be produced in the lower Z collision partner via rotational coupling ($\partial/\partial\theta$ matrix element) of a vacancy in the $2p\pi$ molecular orbital (correlating to the L shell of the higher Z partner) to the $2p\sigma$ molecular orbital (correlating to the K shell of the lower Z partner). Further transfer of the vacancy from the $2p\sigma$ orbital to the $1s\sigma$ orbital (correlating to the K shell of the higher Z partner) via radial coupling ($\partial/\partial r$ matrix element) may produce a K vacancy in the higher Z collision partner.⁴⁹ Such coupling could account for

K-vacancy transfers to the target from projectiles with and without K vacancies. This could represent a major contribution for heavy projectiles since the multiple ionization associated with these projectiles would produce many L-shell vacancies in the target.

APPENDIX B

In the case where the incident ion is stopped in the target, the thick target x-ray production cross section is given by⁵⁰

$$\sigma_X(E) = \frac{1}{n} \frac{dY(E)}{dE} S(E) + \frac{1}{n} \mu Y(E) \quad ,$$

where n is the target atom density in atoms/gm, $Y(E)$ is the number of x rays per incident ion at energy E , $S(E)$ is the stopping power in keV cm²/gm, μ is the x-ray mass absorption coefficient in cm²/gm, and $\sigma_X(E)$ is the x-ray production cross section in cm²/atom. The uncertainties associated with thick target data are primarily due to unreliable values for $dY(E)/dE$ and $S(E)$. Such problems can be eliminated by using thin, transmission mounted targets. For this case the number of target K x rays emitted is given by

$$Y = \sigma_X \rho N_P \quad ,$$

where ρ is the area target density in atoms/cm², and N_P is the number of incident ions. It is assumed in this expression that the target x rays are emitted isotropically.⁵¹

The number of x rays detected, Y_X , is given by the product of the number of x rays emitted, Y , and the x-ray detector efficiency, ϵ . Using this in the previous equation yields

$$\sigma_X = \frac{Y_X}{N_P} \frac{1}{\rho} \frac{1}{\varepsilon} .$$

The number of target atoms/cm², ρ , can be determined by monitoring the number of projectiles which undergo Rutherford scattering, Y_P , and using the following equation

$$Y_P = \rho N_P \Omega \frac{d\sigma}{d\Omega} ,$$

where $d\sigma/d\Omega$ is the differential Rutherford scattering cross section in the laboratory frame of reference. Substituting the value of ρ from this equation into the expression for σ_X gives

$$\sigma_X = \frac{Y_X}{Y_P} \Omega \frac{d\sigma}{\varepsilon d\Omega} ,$$

where it has been assumed that the scattering of the projectiles is totally Rutherford. In addition the differential scattering cross section in the laboratory frame of reference, $d\sigma/d\Omega$ in barns/sr, is given by

$$\frac{d\sigma}{d\Omega} = 1.2965 \times 10^{-3} \left(\frac{Z_1 Z_2}{E} \right)^2 \frac{1}{\sin^4(\theta/2)} \left(1 - 2 \left(\frac{M_1}{M_2} \right)^2 \sin^4(\theta/2) \right) ,$$

where Z_1 , M_1 , Z_2 , and M_2 are the atomic number and mass number of the projectile and target respectively, E is the projectile energy in MeV, and θ is the laboratory angle of the scattering detector.

APPENDIX C

Using notation taken from Allison²⁴ where

$$a = -(\sigma_{01} + \sigma_{12} + \sigma_{21}) \quad ,$$

$$b = (\sigma_{01} + \sigma_{21}) \quad ,$$

$$c = (\sigma_{10} - \sigma_{20}) \quad ,$$

$$d = -(\sigma_{01} + \sigma_{02} + \sigma_{20}) \quad ,$$

and

$$D = ad - bc \quad ,$$

the equilibrium fractions can be written as

$$F_{1\infty} = (b\sigma_{20} - d\sigma_{21})/D \quad ,$$

$$F_{2\infty} = \{ \sigma_{20}(a - b) + d(a + \sigma_{21}) - c(b + \sigma_{21}) \} / D \quad ,$$

and

$$F_{0\infty} = (c\sigma_{21} - a\sigma_{20})/D \quad .$$

Similarly with

$$q = \{(d - a)^2 + 4bc\}^{1/2}/2$$

and

$$s = (d - a)/2 \quad ,$$

$P(i,j)$ and $N(i,j)$ can be written as

$$\frac{P(0,1)}{N(0,1)} = \frac{+}{-} \{ bF_{2\infty} + (b + s \mp q)F_{1\infty} \} / 2q \quad ,$$

$$\frac{P(1,1)}{N(1,1)} = \frac{-}{+} \{ (s \mp q)(1 - F_{1\infty}) + bF_{0\infty} \} / 2q \quad ,$$

$$\frac{P(2,1)}{N(2,1)} = \frac{+}{-} \{F_{1\infty}(s \mp q) - bF_{0\infty}\}/2q \quad ,$$

$$\frac{P(i,2)}{N(i,2)} = -\{\frac{P(i,1)}{N(i,1)} (b + s \mp q)\}/b \quad ,$$

and

$$\frac{P(i,0)}{N(i,0)} = \{\frac{P(i,1)}{N(i,1)} (s \mp q)\}/b \quad .$$

Finally $f(\sigma_{if})$ and $f'(\sigma_{if})$ can be written as

$$f(\sigma_{if}) = (2q - a - d)/2$$

and

$$f'(\sigma_{if}) = (2q + a + d)/2 \quad .$$

APPENDIX D

The simultaneous fits of the data were performed using the following least squares fitting program. The program is written in FORTRAN IV compatible with a Digital Equipment Corporation PDP-15 computer. The program requires initial estimates of nine parameters which are given as follows:

1. σ_{K0}
2. α
3. β
4. σ_{01}
5. σ_{10}
6. σ_{02}
7. σ_{12}
8. σ_{21}
9. σ_{20}

The program will then vary any number of parameters, NPV, for any number of iterations, ITMAX. Options for tabulation and/or plotting of the fit are available.

```

C      PROGRAM XRAYFT
C      MAIN PROGRAM FOR LEAST SQUARES
C      FITTING ROUTINE TO SPECTRA
C      USE WITH SUBPROGRAMS DATA,MATINV,HELPRD,FUNCT1
C
      REAL INAME
      DIMENSION FILEIN(2),PLOT(121)
      COMMON Y0(90),YC(90),Y01(90),IYA(90)
      COMMON B(10),IPAR(10),P(10),G(10),A(10,10)
      COMMON INAME(16),DUMMY(150)
      COMMON NDAT,NPAR,NPV,ITMAX,IFUN,NLOES,NPRT
      EQUIVALENCE(PLOT(1),DUMMY(1))
      CHIMAX=1.E50
1      IFUN=0
2      CALL DATA
      ITER=0
      DEG=NDAT-NPV
      IF (DEG) 6,6,20
6      WRITE(2,/)
7      FORMAT(10H OVER SPEC)
      DEG=1.0
20     CHISQ=CHIMAX
      WRITE(2,3) INAME
5      FORMAT(1H16A5//9X18H INITIAL PARAMETER )
      WRITE(2,4)(I,B(I),I=1,NPAR)
4      FORMAT ( 9X, 15, 1PE10.3 )
      WRITE(2,5)(IPAR(I),I=1,NPV)
5      FORMAT(5H VARY,15I3)
      CALL TIME(MINUTE,ISECOND,IOFF)
10     ITER=ITER+1
      CHIL=CHISQ
      CHISQ=0.
      DO 200 I=1,NDAT
      CALL FUNCT(I)
      TMP=Y0(I)-YC(I)
      CHISQ=CHISQ+TMP*TMP/(Y0(I)+1.)
200    CONTINUE
      WRITE(2,201)CHISQ
201    FORMAT(10X,8H CHISQ =,1PE13.5)
220    IF (ITER-ITMAX) 230,230,1100
230    TMP=CHISQ-CHIL
      IF (ABS(TMP)-0.001) 1000,1000,240
240    IF (TMP) 260,260,250
250    IF (ITER-3) 260,260,1200
260    DO 271 I=1,NPV
      G(I)=0.
      DO 270 J=1,NPV
      A(I,J)=0.
270    CONTINUE
271    CONTINUE
      DO 100 I=1,NDAT
      TMP=YC(I)
      DO 110 III=1,NPV
      J=IPAR(III)
      PTMP=B(J)
      DELP=PTMP*0.001

```

```

      IF (DELP) 102,101,102
101  DELP=0.0001
102  B(J)=PTMP+DELP
      CALL FUNCT(I)
      B(J)=PTMP
      P(III)=(YC(I)-TMP)/DELP
110  CONTINUE
      YC(I)=TMP
      TMP=YC(I)-TMP
      DO 121 JJ=1,NPV
      PTMP=P(JJ)/(YC(I)+1.)
      G(JJ)=G(JJ)+TMP*PTMP
      DO 120 II=JJ,NPV
      A(II,JJ)=A(II,JJ)+P(II)*PTMP
      A(JJ,II)=A(II,JJ)
120  CONTINUE
121  CONTINUE
100  CONTINUE
      CALL MATINV
      IF (NLOES) 1300,300,1300
300  DO 310 I=1,NPV
      J=IPAR(I)
      B(J)=B(J)+G(I)
310  CONTINUE
      WRITE(1,21)ITER
21  FORMAT(' ITER NO.'I5)
      WRITE(1,22)(I,B(I),I=1,NPAR)
22  FORMAT(1X,I5,1PE10.3)
      GO TO 10
1100 WRITE(2,1101)
1101 FORMAT(9H ITER OUT)
      GO TO 1010
1000 WRITE(2,1001)
1001 FORMAT(8H OK EXIT)
1010 CHISQ=CHISQ/DEG
      WRITE(1,1012)CHISQ
      WRITE(2,1012)CHISQ
1012 FORMAT(6X,11HCHISQ/DEG =,1PE13.5)
      WRITE(2,1011)
1011 FORMAT(13H FINAL PARAMS,10X,5HVALUE,5X,25HSTAT ERROR
1R)
      CHISQ=SQRT(CHISQ)
      DO 1020 I=1,NPAR
      G(I)=0.0
1020 CONTINUE
      DO 1030 I=1,NPV
      J=IPAR(I)
      G(J)=SQRT(ABS(A(I,I)))
1030 CONTINUE
      DO 1040 I=1,NPAR
      TMP=G(I)*CHISQ
      WRITE(2,1013) I,B(I),G(I),TMP
1013 FORMAT(10X,I5,3(1PE15.5))
1040 CONTINUE
      SPI=1.2533141
      WRITE(2,1014)
1014 FORMAT(14X,' CHANNEL NO.          AREA'9X'ERROR')

```

```

      DO 1302 I=3,NPAR,3
      DELP=SPI*(B(I)+G(I+2)+B(I+2)+G(I))
      TMP=SPI*B(I)+B(I+2)
      WRITE(2,1303)B(I+1),TMP,DELP
1303  FORMAT(14X,3(G15.7))
1302  CONTINUE
      IOFF=1
      WRITE(2,4000)MINUTE,ISECND
4000  FORMAT($ ELAPSED TIME: $I3$MINUTES$I3$SECONDS$)
      IF(NPRT)400,401,401
401  WRITE(2,211)
211  FORMAT(14X,1HX,11X,4HDATA,10X,5H  FIT,9X,9HTHICKNESS)
      DO 213 I=1,NDAT
      XII=I
      YDII=YD(I)
      YCII=YC(I)
      YBII=YD(I)
      YB=YD(I)/9.474E-09
213  WRITE(2,212)XII,YDII,YCII,YBII,YB
212  FORMAT(5(1PG15.5))
400  CONTINUE
      IF(NPRT+2)801,801,403
403  CONTINUE
      IF(NPRT)402,801,402
402  WRITE(2,1400)INAME
1400  FORMAT(1H116A5///)
      BIG=0.0
      DO 9100 I=1,NDAT
      IF(BIG-YD(I)) 9110,9120,9120
9110  BIG=YD(I)
9120  IF(BIG-YC(I)) 9130,9140,9140
9130  BIG=YC(I)
9100  CONTINUE
      BIG=90./BIG
      DO 9000 I=1,NDAT
      DO 9900 J=1,121
      PLOT(J)=1H
9900  CONTINUE
      J=YC(I)*BIG
      PLOT(J)=1H*
      J=YD(I)*BIG
      PLOT(J)=1H0
      WRITE(2,800)I,PLOT
8000  CONTINUE
800  FORMAT(1X,I3,2H ^,121A1///)
801  CONTINUE
      WRITE(1,500)
500  FORMAT($ TYPE -1 FOR INIT. PARAM., 0 FOR NEW DATA,$/
      1$ +1 FOR NEW VARIABLES$)
      READ(1,501)IFUN
501  FORMAT(I3)
      GO TO 2
1200  WRITE(2,1201)
1201  FORMAT(7H CHI UP)
      DO 1210 I=1,NPV
      J=IPAR(I)
      B(J)=B(J)-G(I)

```



```
1210 CONTINUE  
    ITER=ITMAX  
    GO TO 10  
1300 WRITE(2,1301)  
1301 FORMAT(9H SINGULAR)  
    IF(ITER-1) 2,2,1010  
    END
```

C
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SUBPROGRAM TO XRAYFT
READS IN SPECTRA TO BE FIT

75

```

SUBROUTINE DATA
  REAL INAME
  DIMENSION FILEIN(2),C(3)
  COMMON YD(90),YC(90),YD1(90),IYA(90)
  COMMON B(10),IPAR(10),P(10),G(10),A(10,10)
  COMMON INAME(16),DUMMY(150)
  COMMON NDAT,NPAR,NPV,ITMAX,IFUN,NLOES,NPRT
  IF(1FUN) 200,100,300
100  WRITE(1,1000)
1000  FORMAT(6H TITLE )
  READ(1,101)INAME
  101  FORMAT(16A5)
  WRITE(1,1002)
1002  FORMAT(' NPRT:1=BOTH,0=TABLE,-1=PLOT,-2=NEITHER')
  WRITE(1,1001)
1001  FORMAT(35H TYPE NDAT, CR, NPAR, CR, NPRT, CR )
  READ(1,203)NDAT,NPAR,NPRT
  203  FORMAT(I3)
  WRITE(1,400)
  400  FORMAT(' TYPE 1 FOR TAPE, -1 FOR HAND ENTERED DATA')
  READ(1,401)NT
  401  FORMAT(I3)
  IF(NT) 402,403,403
  403  CONTINUE
  WRITE(1,404)
  404  FORMAT(10H FILE NAME)
  READ(1,405)FILEIN
  405  FORMAT(A5,A4)
  CALL FSTAT(3,FILEIN,NF)
  IF(NF.EQ.-1) GO TO 410
  WRITE(1,411)
  411  FORMAT(' FILE NOT FOUND')
  GO TO 403
  410  CALL SEEK(3,FILEIN)
  DO 406 I=1,NDAT
  READ (3)(C(K), K=1,3)
  YD(I)=C(1)
  YD1(I)=C(2)
  IYA(I)=C(3)
  406  CONTINUE
  GO TO 7
  402  CONTINUE
  DO 7 I=1,NDAT
  WRITE(1,6)
  6  FORMAT(' TYPE CROSS SECTION, THICKNES AND "A"')
  READ(1,) YD(I),YD1(I),IYA(I)
  7  CONTINUE
  3000  FORMAT(34H INITIAL PARAMETERS, ONE TO A LINE)
  200  WRITE(1,3000)
  READ(1,204)(B(I),I=1,NPAR)
  204  FORMAT(E10.3)
  WRITE(1,1)
  1  FORMAT(' TYPE 1 IF ANY PARAMETERS ARE INCORRECT')

```

```
      READ(1,203)N
      IF(N.EQ.1)GO TO 2
      GO TO 300
2     WRITE(1,3)
3     FORMAT(' TYPE PAR. NO. AND NEW VALUE(13,E10.3)')
5     READ(1,4)N,TEMP
4     FORMAT(13,E10.3)
      IF(N.EQ.0)GO TO 300
      B(N)=TEMP
      GO TO 5
300    WRITE(1,4000)
4000   FORMAT(13H NEW CONTROLS /29H ITMAX,NPV,IPAR(I),I=1,NPV /
           1 14H ONE TO A LINE )
      READ(1,203)ITMAX,NPV,(IPAR(I),I=1,NPV)
      RETURN
      END
```

C
C
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C

SUBPROGRAM TO XRAYFT
INVERTS MATRIX A

77

```

SUBROUTINE MATINV
  REAL INAME
  DIMENSION IPIVOT(33),INDEX(33,2),PIVOT(33)
  DIMENSION FILEIN(2),PLUT(121)
  COMMON YQ(90),YC(90),YD1(90),IYA(90)
  COMMON B(10),IPAR(10),P(10),G(10),A(10,10)
  COMMON INAME(16),DUMMY(150)
  COMMON NDAT,NPAR,NPV,IIMAX,IFUN,NLOES,NPRT
  EQUIVALENCE (IROW,JROW),(ICOLUMN,JCOLUMN),(AMAX,T,SWAP)
  NLOES=0
  DO 20 J=1,NPV
20  IPIVOT(J)=0
  DO 550 I=1,NPV
  AMAX=1.0E-30
  IANZ=0
  DO 105 J=1,NPV
  IF (IPIVOT(J)-1) 60,106,60
60  DO 100 K=1,NPV
  IF (IPIVOT(K)-1) 80,99,71
71  NLOES=1
  RETURN
80  IF (ABS(AMAX)-ABS(A(J,K))) 84,99,99
84  IANZ=IANZ+1
  IROW=J
  ICOLUMN=K
  AMAX=A(J,K)
99  CONTINUE
100 CONTINUE
106 CONTINUE
105 CONTINUE
  IF (IANZ) 71,71,110
110 IPIVOT(ICOLUMN)=IPIVOT(ICOLUMN)+1
  IF (IROW-ICOLUMN) 150,260,150
150 DO 200 L=1,NPV
  SWAP=A(IROW,L)
  A(IROW,L)=A(ICOLUMN,L)
200 A(ICOLUMN,L)=SWAP
  SWAP=G(IROW)
  G(IROW)=G(ICOLUMN)
  G(ICOLUMN)=SWAP
260 INDEX(I,1)=IROW
  INDEX(I,2)=ICOLUMN
  PIVOT(I)=A(ICOLUMN,ICOLUMN)
  A(ICOLUMN,ICOLUMN)=1.0
  DO 350 L=1,NPV
350 A(ICOLUMN,L)=A(ICOLUMN,L)/PIVOT(I)
  G(ICOLUMN)=G(ICOLUMN)/PIVOT(I)
  DO 551 L1=1,NPV
  IF (L1-ICOLUMN) 400,552,400
400 T=A(L1,ICOLUMN)
  A(L1,ICOLUMN)=0.0
  DO 450 L=1,NPV
450 A(L1,L)=A(L1,L)-A(ICOLUMN,L)*T

```

```
G(L1)=G(L1)-G(ICOLUM)*T
552   CONTINUE
551   CONTINUE
550   CONTINUE
      DO 710 I=1,NPV
      L=NPV+1-I
      IF(INDEX(L,1)-INDEX(L,2)) 630,709,630
630   JROW=INDEX(L,1)
      JCOLUM=INDEX(L,2)
      DO 705 K=1,NPV
      SWAP=A(K,JROW)
      A(K,JROW)=A(K,JCOLUM)
      A(K,JCOLUM)=SWAP
705   CONTINUE
709   CONTINUE
710   CONTINUE
      RETURN
      END
```

SUBPROGRAM TO XRAYFT
 CALCULATES FITTING FUNCTION (ALLISON)
 ALLOWS UP TO NINE VARIABLES TO BE FIT

C
 C
 C
 C
 C

5

10

20

30

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SUBROUTINE FUNCT(I)
REAL INAME
DIMENSION FILEIN(2)
COMMON Y0(90),YC(90),Y01(90),IYA(90)
COMMON B(10),IPAR(10),P(10),G(10),A(10,10)
COMMON INAME(16),DUMMY(150)
COMMON NDAT,NPAR,NPV,ITMAX,IFUN,NLDES,NPRT
DO 5 J=1,NPAR
  B(J)=ABS(B(J))
CONTINUE
  A1=B(4)+B(6)
  B1=B(5)+B(7)
  G1=B(9)+B(8)
  A2=-(B1+B(8))
  B2=B(4)-B(8)
  F2=B(5)-B(9)
  G2=-(A1+B(9))
  Q=(SQRT(((ABS(G2-A2))**2.)+4.+(B2+F2)))/2.
  S1=-(A2+G2)
  S2=(G2-A2)/2.
  D=(A2*G2)-(B2+F2)
  F0I=((B1*B(9))+(B(5)*B(8)))/D
  F1I=((A1*B(8))+(B(4)*B(9)))/D
  F2I=((B(9)*(A2-B2))+(G2*(A2+B(8)))-(F2*(B2+B(8))))/D
  T1=(B2+S2+Q)/B2
  T2=(B2+S2-Q)/B2
  T3=(S2+Q)/B2
  T4=(S2-Q)/B2
  IF (IYA(I).EQ.1) GO TO 10
  IF (IYA(I).EQ.2) GO TO 20
  P1=((B2+F2I)+((B2+S2-Q)*F1I))/(Q*2.)
  X1=-((B2*F2I)+((B2+S2+Q)*F1I))/(Q*2.)
  GO TO 30
10  P1=-((S2-Q)*(1.-F1I)+(B2*F0I))/(Q*2.)
    X1=((S2+Q)*(1.-F1I)+(B2*F0I))/(Q*2.)
    GO TO 30
20  P1=((F1I*(S2-Q))-(B2*F0I))/(Q*2.)
    X1=-((F1I*(S2+Q))-(B2*F0I))/(Q*2.)
30  P2=-P1*T1
    X2=-X1*T2
    P0=P1*T3
    X0=X1*T4
    E1=(EXP(Y01(I)*(Q-(S1/2.)))-1.)/(Y01(I)*(Q-(S1/2.)))
    E2=(EXP(-Y01(I)*(Q+(S1/2.)))-1.)/(Y01(I)*(Q+(S1/2.)))
    Y0=F0I+(P0*E1)-(X0*E2)
    Y1=F1I+(P1*E1)-(X1*E2)
    Y2=F2I+(P2*E1)-(X2*E2)
    YC(I)=B(1)*(Y0+(B(2)*Y1)+(B(3)*Y2))
RETURN
END

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