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Double-Scattering Mechanism to Account for the Si *K*-X-Ray Yields Observed during Argon-Ion Bombardment of Silicon

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Si K x rays are observed when solid Si is bombarded by 160–260-keV Ar^{++} ions. The production of such x rays is interpreted in terms of the Fano-Lichten model, and a double-scattering mechanism whereby Si K vacancies are produced by electron promotion to an Ar $L_{2,3}$ vacancy formed in a prior collision.

The Fano-Lichten[1] model has been used extensively to explain the copious production of inner-shell vacancies in collisions between heavy ions up to energies of the order of 500 keV. In this model, the projectile-target system is represented as a temporarily formed diatomic molecule characterized by the diabatic, independent-particle orbitals and energies. When the energy level of a molecular orbital (MO) containing a vacancy crosses, or is degenerate with, an initially lower energy level corresponding to a filled orbital, the vacancy can be transferred to this second orbital. After the collision partners separate, the transferred vacancy becomes an atomic inner-shell vacancy. This model is in accord with a large variety of experimental data.[2]

We have observed Si K x-rays produced by bombarding solid silicon with Ar^{++}. Here, the Si K vacancies cannot be produced by the promotion mechanism, since the MO which correlates with the Si K level crosses only the MO's which correlate with the *filled* $2s$ and $2p$ levels of Ar^{++}. In view of the previous successes of the Fano-Lichten model, it is useful to attempt an interpretation of this result within the context of the model. This suggests immediately that the Si K vacancies are formed by electron promotion to previously formed Ar $L_{2,3}$ vacancies. An interpretation of the data in terms of such a double-scattering mechanism requires a theory relating the observed x-ray yields to the Ar $L_{2,3}$ and Si K production cross sections. The validity of the double-scattering interpretation can then be assessed on the basis of the reasonableness of the cross section thereby deduced.

Pure silicon targets (Monsanto p-type polished slices; resistivity, 5–10 Ω cm) were subjected to bombardment by Ar^{++} ions over the energy range 120–260 keV. The x-rays thereby produced, viz., Ar L (~220 eV) and Si K (~1740 eV) were detected by an end-window x-ray proportional counter[3] incorporating a 6-μm aluminized Mylar window. The high geometrical collection efficiency of this instrument enabled the ion dose to be kept to a minimum, viz., 15 μC at each energy, while yielding good counting statistics—for example, at 260 keV the Ar L and Si K yields were typically 240 000 and 71 500, respectively. It is important, in studies of this nature, that the heavy-ion dose be kept to a minimum, so as to avoid projectile buildup in the target, thus causing the Ar L yield to be magnified. Therefore, as a further precaution, six identical silicon slices were mounted on a wheel in the target chamber, and a new area of silicon was exposed to the beam at each energy. In the course of this work we were surprised to observe an additional unexpected x ray in the spectrum. This had an energy of ~950 eV and exhibited a threshold at ~80 keV. However, since it is irrelevant to the present discussion, it will not be considered further at this stage. A more complete discussion of this line will be presented elsewhere.[4]

It is a common practice to use doubly charged ions to extend the effective energy range of the projectiles. This is based on the assumption that the x-ray yields from singly and doubly charged ions of the same effective energy will be identical. However, it has been noticed recently[5] that under certain conditions this assumption may not be valid. Thus to avoid any potential confusion, only the results obtained for doubly charged ions will be used here.

Naturally, the observed x-ray yields must be corrected for loss in intensity on passing through the 6-μm Mylar window. This is particularly important for the soft Ar L x rays. We actually measured their transmission, and thereby obtained a correction factor of 226. This allowed us to deduce a mass absorption coefficient of 6200 cm^2/g, which corresponds to a wavelength of 56.5 Å[6]; the wavelength of Ar L_3M_1 is listed as 56.3 Å, with a probable error of 1 in the last digit.[7] It should be noted that in dealing with such ultrasoft x rays it is unwise to estimate the mass absorption coefficient, because the correction factor thereby obtained may be seriously in error. For example, if a mass absorption coefficient of 6100 had been used (based on a value of 56.0 Å for the Ar L wavelength), the correction factor thereby deduced would have been only 166!

In order to relate the measured yields to the vacancy production cross sections, the theory of double scattering in a thick target must be considered. When the incident beam of ions in their initial state enters the solid, the ions continuously change states by collisional excitation followed by Auger and radiative decay. At any point in the solid the beam will contain a certain fraction of ions with an inner-shell vacancy. We denote this state by the index 1. To determine the x-ray yield produced by collisions of beam ions in state 1 with target atoms, we need only calculate the fraction f of ions in this state and insert the fraction into the usual expression for x-ray yields in thick targets.[8] This fraction in general depends upon both the range R of the incident ions, and the residual range R' of the ions at some point in the solid. In the application employed here it is sufficient to approximate the fraction $f(R, R')$ by the equilibrium fraction $f(R')$ for particles with a residual range R', neglecting the dependence upon R.[9] Then $f(R, R')$ is simply[10]

$$f(R, R') \approx f(R') = n\sigma_1(R')v(R')\tau_1, \tag{1}$$

where n is density of target atoms per unit volume, $\sigma_1(R')$ is the cross section for exciting the incident ions to state 1 when they have a residual range R', $v(R')$ is the velocity of the ions with residual range R', and τ_1 is the lifetime of state 1. It is useful here to estimate $f(R')$ to see if the fraction of Ar ions with Ar $L_{2,3}$ vacancies is large enough to account for the observed Si K x-ray yields. The 260-keV Ar ions have a velocity of approximately $v = 1.13\times10^8$ cm/sec, the density of silicon is 0.5×10^{23} atoms/cm^3, while McGuire[11] calculates a value of 4×10^{-15} sec for τ_1. Taking σ_1 approximately equal to a fraction, say $\frac{1}{3}$, of the geometric cross section for the Ar L_2 shell, we find $f(R') \approx 0.05$. Since the ratio of the Ar L_2 and Si K fluorescent yields is[11] 3.67×10^{-3}, while the ratio of the Ar L_2- and Si K-shell geometric cross sections is 16, we see that $f\approx 0.05$ corresponds to nearly equal Ar L and Si K x-ray yields and is sufficient to account for the observed ratio of yields, assuming that the yields are approximately proportional to the cross section times the fluorescent yields. Thus we conclude that the postulated double-scattering mechanism is tenable, and we will use this interpretation to extract a cross section for the transfer of an Ar $L_{2,3}$ vacancy to a Si K shell from the experimental data. We shall see that the resulting cross section is in accord with the expectations of the Fano-Lichten model.

Inserting the fraction (1) into Lewis, Simmons, and Merzbacher's[8] expression for the cross section σ_2 for producing a target atom in state 2 when the incident ion is in state 1, we obtain

$$dY_2/dE + \mu_2 Y_2\, dR/dE = n\sigma_2(E)\omega_2(E)[n\sigma_1(E)v(E)\tau_1(E)]\,dR/dE, \tag{2}$$

where Y_2 is the yield of x rays from the target atom in state 2, μ_2 is the corresponding linear absorption coefficient, dE/dR is the stopping power, and ω_2 is the fluorescent yield of target atoms in state 2. Similarly the cross section for producing projectile ions in state 1 is given in terms of the yield Y_1 of x rays from the decay of state 1 according to

$$dY_1/dE + \mu_1 Y_1 dR/dE = n\sigma_1(E)\omega_1(E)\, dR/dE. \tag{3}$$

Solving Eqs. (2) and (3) for $\sigma_2(E)$ gives

$$\sigma_2(E) = [dY_2/dE + \mu_2 Y_2 dR/dE][dY_1/dE + \mu_1 Y_1 dR/dE]^{-1}\omega_1(E)[\omega_2(E)\tau_1(E)v_1(E)n]^{-1}. \tag{4}$$

Equation (4) has been used to calculate σ_2, where the subscript 2 denotes a silicon atom with a K-shell vacancy, from the measured Si K- and Ar L-x-ray yields. The measured Ar L yield is the sum of the $L_{2,3}$ and L_1 yields. In the Fano-Lichten model, the L_1 yield should be small compared with the $L_{2,3}$ yield. In the analysis it has been supposed that no L_1 x rays are produced. This approximation may result in an error of at most 20% in the calculated Si K cross sections. The following table lists the constants used in Eq. (4) and the sources from which they were taken.

Ar $L_{2,3}$ radiative rate (Ref. 11)	0.58×10^{11}/sec
$\omega_{\mathrm{Si}\,K}$ (Ref. 13)	5.14×10^{-2}
$\mu_{\mathrm{Ar}\,L}$ (Ref. 6)	5.60×10^{4} cm/g
$\mu_{\mathrm{Si}\,K}$ (Ref. 6)	3.25×10^{2} cm^2/g

Here we note that ω_1/τ_1 in Eq. (4) equals the Ar $L_{2,3}$ radiative rate. The stopping power was taken from the tables of Johnson and Gibbons.[12]

The cross section for production of Si K vacancies by collision with argon ions having an $L_{2,3}$ vacancy is shown in Fig. 1. The curve shows an onset at an energy approximately equal to the energy required to bring an argon atom and a silicon atom together to a separation equal to the Si K-shell radius. This is in agreement with the Fano-Lichten theory. Further, the cross section rises an order of magnitude over an energy range of 80 keV. This rapid rise is characteristic of the promotion mechanism. The cross section deduced is considerably smaller than geometric and has not yet saturated in the energy range up to 260 keV. In the Fano-Lichten model, a leveling off of the cross section at an impact velocity which is roughly twice the threshold value is expected. Here, the maximum impact velocity is only 50% greater than the threshold value and therefore this small cross section is to be expected. The results are consistent with the Fano-Lichten model in the energy range covered by the experiment.

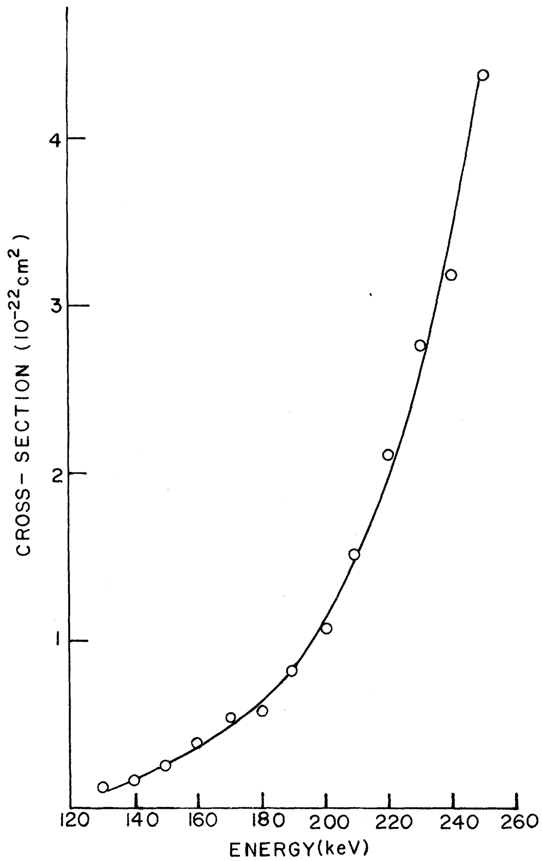

FIG. 1. Cross section for transferring an Ar L_2 vacancy to a Si K shell.

It is concluded that double scattering can account for a significant x-ray yield for inner shells not ordinarily excited in single collisions involving keV ions.

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Deduction of Continuum Potentials from Planar Channeling

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A new method for determining planar continuum potentials from planar channeling data has been developed. Preliminary experiments have been done for 1.8-MeV α particles in [111] gold planar directions from which the continuum potential has been deduced.

During the past several years the experimental observation of fine structure in the energy loss of planar-channeled particles having specific trajectories in transmission through thin crystals has been exploited by several authors[1-7] in an attempt to characterize the detailed motion of the penetrating particle and associated phenomena. Of particular importance in such studies is the planar continuum potential[8,9] since this function serves as the starting point for more detailed experimental and theoretical investigations of channeled particle properties. In this Letter we report on a new and direct method of obtaining the continuum potential from the analysis of planar channeling data.

This approach to determing the continuum potential is based upon the realization that for a symmetric one-dimensional anharmonic oscillator of known mass, knowledge of the oscillation period as a function of the total oscillator energy is sufficient to uniquely deduce the potential function responsible for the motion.[10] The pioneering work of Datz *et al.*[3] showed how the wavelengths of the transverse motion of planar-channeled particles can be determined in a straightforward way, from which the period of the transverse oscillations follows directly. In this work we show a direct method to extract the energy of the transverse motion, which together with the wavelength measurement provides enough information to uniquely determine the continuum potential necessary to describe the transverse motion of the channeled particle.

Briefly reviewing the experimental procedure, after the planar-channeled beam emerges from a thin crystal, it is energy analyzed with a masked solid-state detector having an angular resolution of $\sim 2.5\times 10^{-7}$ sr, positioned in line with the incident beam. Under these conditions the particles recorded by the detector are mainly those whose trajectories have undergone an integral number of wavelengths in the crystal.[3] If the detector has sufficient energy resolution, particles having different numbers of wavelengths in the crystal can be distinguished since each has a characteristic energy loss rate, corresponding to different amplitudes of oscillation in the channel. A schematic illustration of the trajectory selection principle is shown in Fig. 1. (As can be seen from this figure, the wavelength of the motion of a particular group can be determined by experimentally increasing the crystal thickness L until another group of an equal energy loss rate is found. The increase in thickness will be 1 wavelength for those groups.[3])

For this detector geometry, changing the angle between the crystal plane and the incident beam, keeping the crystal thickness along the beam direction constant, has the effect of changing the populations of the various detected wavelength