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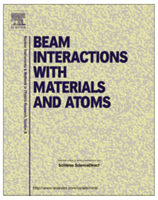

BEAM INTERACTIONS WITH MATERIALS AND ATOMS

Werner Brandt legacy to PIXE: Past and present perspectives

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ABSTRACT

Inner-shell ionization cross sections used in Particle-Induced X-ray Elemental (PIXE) analyses are routinely calculated in the ECPSSR [W. Brandt, G. Lapicki, Phys. Rev. A 23 (1981) 1717–1729] theory and/or semiempirical formulas scaled to that theory. Thirty years after the passing of Werner Brandt, with recognition of his seminal contributions to other research on positron physics and stopping power problems, the work and articles that progressed into the ECPSSR theory for inner-shell ionization by protons and heavier ions are recalled as Brandt's past legacy to the PIXE community. Applications of the ECPSSR and its evolution into the ECUSAR [G. Lapicki, Nucl. Instr. Meth. B 189 (2002) 8–20] theory over the last three decades are reviewed with perspectives on Brandt's present legacy.

1. Work of Brandt and co-workers prior to 1983

1.1. Early work prior the initiation of inner-shell ionization theory and x-ray production experiments in 1966

Already in his first publication, on calculation of intermolecular force constants from polarizabilities [1], Brandt showed superb ability to scale the data so as to extract these constants in the Lennard–Jones potential for a variety of molecules. His work at DuPont followed with papers on stopping power [2], compressibilities of high-polymers [3], and a seminal article on positronium decay in molecular substances [4]. His first NYU article on Bose–Einstein condensation of excitons [5] was followed by a series of papers on atomic collective response [6] and a paper on the effect of proton channeling on x-ray production in crystals [7], which inspired Brandt to pursue a new field of research that was to become his legacy to the PIXE community.

A New York Times obituary noted, inter alia, that Brandt directed New York University's Radiation and Solid State Laboratory which since the early 1960's had been an interdisciplinary venture that had used biochemistry and physical chemistry, as well as physics, to probe the interaction of matter and energy [8]. A program from his memorial service [9] listed and elaborated on three key areas in which Brandt has excelled during his career as an outstanding original researcher: active and definitive analysis of inner-shell excitations by atomic projectiles, studies of positron annihilation, and stopping powers of charged particles in matter. Aside from a plethora of publications on stopping powers, the titles of informal annual workshops held every January in the 1977–1983 period [10], and continued to this day as the Werner Brandt Workshops, inform and reflect on Brandt's leadership in the field of penetration of charged particles in matter. An obituary [11] describes Brandt's work and in memoriams [12] vividly capture memories about him. While it would be impossible to review all his seminal and multi-facted contributions to physics, this review is written from my perspective as one of Brandt's last students and the next-to-last post doc at the time when the Fig. 1 photo was taken.

1.2. Development of an inner-shell ionization theory and experiments for x-ray production in 1966–1982

After two positron articles [13], Brandt, Laubert, and Sellin initiated the development of an inner-shell ionization theory and measurements of x-ray production cross sections [14]. Without referencing all of circa 200 subsequent articles written by Brandt and coworkers, their chronological review is limited to those works that have become forerunners to and benefactors of the ECPSSR theory [15]. In [14], the first two ingredients of that theory were introduced: (i) the Coulomb deflection factor accounting for deflection of the projectile from a straight-line trajectory and (ii) additional binding to the projectile of the to-be-ejected electron. Both effects increasing with the decreasing projectile velocity result in increasingly smaller cross sections than calculated by the plane-wave Born approximation (PWBA). This was verified by measured K-shell x-ray production cross section in bombardment of $_{12}$Mg and $_{13}$Al by 25–50 keV/amu singly-charged ions of H, ^{3}He, and ^{4}He [14], and further exhibited in the 25–200 keV/amu range with these projectiles for the K-shell data on aluminum [16]. At 25 keV/

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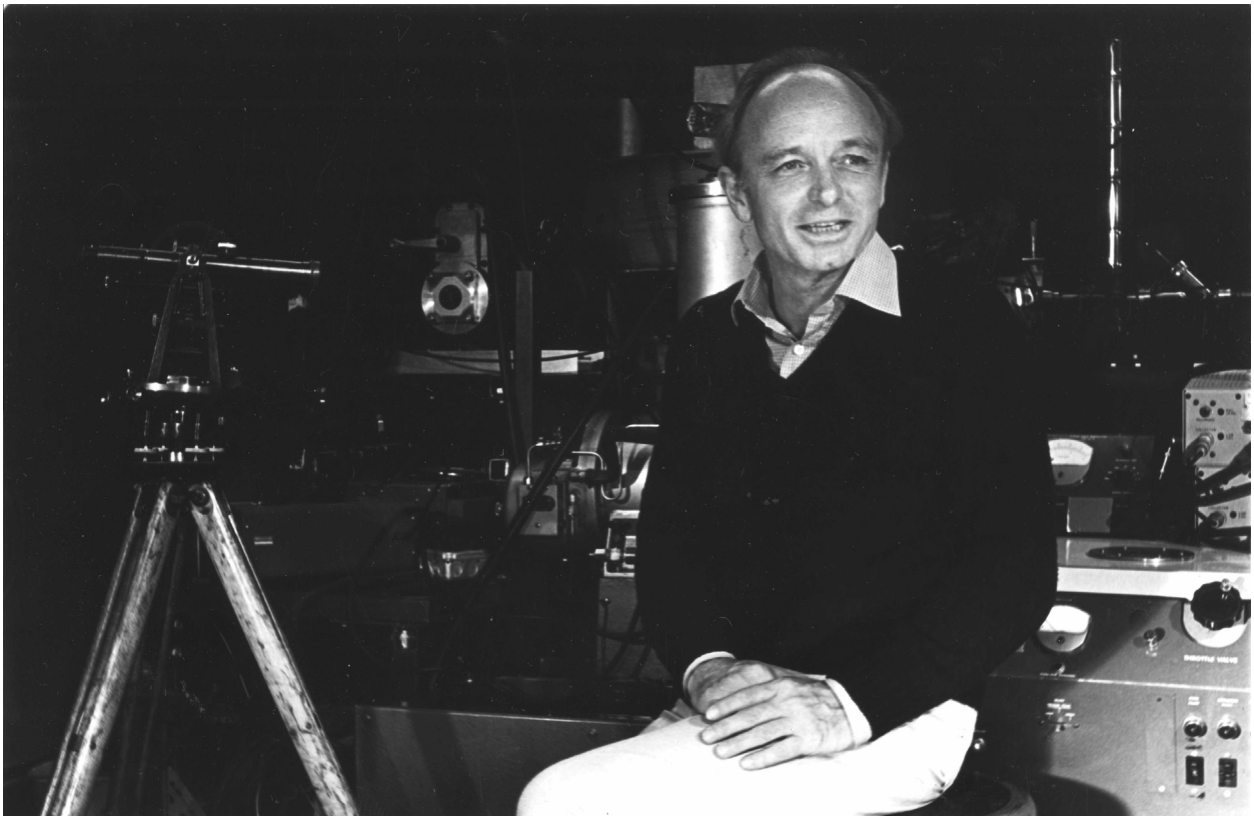

Fig. 1. Werner Brandt (1925–1981). Photo circa 1970's from New York University library archives.

amu, cross sections corrected for the Coulomb deflection and binding effects fell two orders of magnitude below the PWBA results. The argument of the Coulomb deflection factor is proportional to the atomic number Z_1 and inversely proportional to the atomic mass A_1 of the projectile so that the ratio of cross sections obtained with isotopes of the same charge and velocity are a direct measure of that factor. The measured ratios of ^{3}He to ^{4}He cross sections (the isotope effect) indeed confirmed [17] the accuracy of the Coulomb deflection factor proposed in [14]. With the smaller Z_1/A_1 for ^{4}He than for ^{1}H, ratios of their cross sections divided by 4 dictated by Z_1^2 scaling of the PWBA and taken at the same velocity would have been greater than 1 on the sole account of the Coulomb deflection. With the binding to the alpha particles stronger than to protons, these ratios were measured to be less than 1 [16] in excellent agreement with the combined effects of the Coulomb deflection and binding as formulated in [14]. New measurements in an extended 0.1–0.9 MeV/amu range [17] showed these ratios to be greater than 1 at the lowest velocity where the Coulomb deflection dominates over the binding effect. Above 0.5 keV/amu those ratios exceeded 1 which, in analogy with the Z_1^3 effect seen in stopping powers [18], was attributed [17] to a high-velocity/large impact-parameter polarization of the K shell. These findings were confirmed for the K shell of $_{13}$Al and $_{28}$Ni bombarded by 1–7.5 MeV/amu ^{1}H, ^{2}H, ^{3}He, ^{4}He, and ^{7}Li ions [19]. At the first international conference on inner-shell ionization phenomena [20], Brandt reviewed the status of the ionization theory developed for the K shell [14,16–19] and included a figure illustrating its application to the L shell of $_{79}$Au [21].

With scaling of K-shell x-ray production cross sections in appropriate variables corrected for the Coulomb deflection and binding effects [14], the data were shown to follow along a universal curve by as much as two orders of magnitude below the PWBA at the lowest energies [22]. The binding and polarization effects [19,22] were ab initio justified in the perturbed-stationary-state (PSS) formalism [23], and also applied in the analysis of the L-shell data at low velocities [24]. Furthermore, for electron capture they were incorporated in the low-velocity theory and joined with the second-order Born result at high velocities as a part of the thesis [25]. Predictions of that electron capture theory [25,26] were successfully used to explain the projectile-charge dependence observed in K- [27,28] and L-shell ionization [29]. As they were found up to 1975 for $Z_2 = 4–92$ elements, cross sections for K- and L-shell x-ray and Auger-electron production by H, He, and Li ions were tabulated and converted to ionization cross sections that were graphically compared with calculations for inner-shell ionization to the target atom continuum plus by electron capture to unoccupied states on the projectile [25].

With more measurements for the K shell and extension to intermediate velocities, where the ionization come increasingly from projectiles passing outside the K shell so as to polarize and thereby enhance its ionization beyond the Z_1^2 scaling of the PWBA, the agreement between the data and the CPSS theory for direct ionization to the target has been improved [30]. The C stands for the Coulomb deflection and the PSS correction accounts for low-velocity binding and intermediate-velocity polarization effects. With an added R, for inclusion of relativistic effects of the target wave function through a procedure that reproduced numerical calculations for heavy target atoms, the CPSS theory became the CPSSR theory [31]. This procedure has been incorporated [32] in the electron capture theory [25,26]. A Coulomb deflection factor from the Coulomb wave function instead of the plane-wave of the PWBA was obtained as an alternative to the C extracted from semiclassical calculations with hyperbolic and straight-line trajectories [33]. With an upcoming evolution of the CPSSR into the ECPSSR theory that was to account for the projectile's energy loss [15], the Coulomb deflection factor was measured at its, to this day, smallest value obtained in ionization of the K-shell of $_{28}$Ni by 55-keV protons [34] and tabulated for its evaluation in ionization of the K-shell and L-subshells.[35]. K-shell x-ray production cross sections by protons collected and referenced in [15] appeared to be in an overall good agreement with the ECPSSR theory. Data taken from a single reference with 60–150 keV protons for K-shell ionization in $21 < Z_2 < 31$ elements, while two orders of magnitude below the PWBA, fell below the ECPSSR by a factor of two at the lowest velocities [36]; the CPPS showed an equal result since the energy-loss and relativistic effects cancelled each other. M-shell cross sections for ionization by H^+ and He^+ were in good overall agreement with the ECPSSR [37], and – while below the ECPSSR – they tended to fall above the ECPSSR predictions at lowest velocities on heavy target elements [38]. Three decades ago, there were plans for antiproton beams in the 0.1–2 GeV range. In an article [39] that appeared at the time of Brandt's passing – by changing the sign in the arguments of the Coulomb deflection and the PSS functions that he and his coworkers have established for ionization by protons – the differences between antiproton and proton ionization would be insignificant in this energy range while at 1 MeV and below antiproton cross sections were predicted to by greater than proton cross sections by orders of magnitude. Whereas Brandt's past legacy to the PIXE analyses with a reliable ionization theory for protons and light positive ions is evident, one could see how prosperous (orders of magnitude more sensitive) the anti-PIXE would have been if only the particle-antiparticle asymmetry were less skewed toward particles.

2. Present (post 1982) legacy of Brandt to the PIXE field

Inner-shell ionization cross sections serve as an input used in PIXE analysis. Originally and as it still continues, the data have been fitted to polynomials in variables and forms dictated by the binary encounter approximation (BEA) [40]. As noted in [25,41], the BEA is adequate only around the peak in the cross section where the projectile velocity matches the electron velocity in the inner shell. As referenced in [41] various theories could be considered as an alternative to the BEA. However, numerical results of these theories {see Refs. 23–29,31–45 in [41]} have been typically reported for a few proton energies, limited set of target atoms, and with an exception of [42] none of these calculations was done for slow collisions.

Aside from shortcomings of the BEA, it is critical that a validation of any theory rests on a comprehensive comparison with databases that cover a wide area of the projectile energies and target elements. A recent validation of K-, L-, and M-shell with a declaration that "the agreement is good for all shells on the 50 keV–100 MeV range" [43], through a comparison with L-shell measurements taken from a single reference for just one target element over a limited 0.05–2 MeV range is a prime example what should be avoided.

The present legacy of Brandt to PIXE rests on the ECPSSR theory [15] and its modification, ECUSAR [44], for calculation of K-, L-, and M-shell ionization cross sections used in numerous PIXE codes [45]. They provide for reliable analyses that were far less certain in the PIXE works cited in [25]. Since these early references of some four decades ago, the PIXE field has mushroomed as evidenced by a variety of latest applications at the current PIXE conference [46]. It is instructive to cite several examples for similar materials from the past [25] to the present [46] where they continue to be investigated with increased sophistication: (i) from trace element concentration along single hairs to a study of its growth in 1-cm increments to measure chronological changes in the hair's elemental make up for survivors of the 2011 tsunami [47], (ii) from a new tool in forensic science to its exploration versus conventional techniques or an elemental footprint of ammunition manufactured by a specific company [48], (iii) from an observation of plant disease in areas highly contaminated by metals or from a difference between elemental content for green and brown 0.5-cm^2 areas of a maple leaf to quantitative elemental mapping for plants over micro-areas at ppm levels or to confocal- and stereo-PIXE with submicron beams [49], (iv) from an early distinction between pollutants and natural background in urban aerosols to comprehensive longitudinal studies for pollution tracking in Beijing, Mexico City, Debrecen, and across continents or to the same times comparisons between in- and out-door pollutants [50], (v) from one nanogram limits in detection of $Z_2 < 30$ metals for routine PIXE analyses to cellular microanalysis of the elevated levels of $_{28}$Fe as a culprit in Parkinson's disease or in fish liver's melanomacrophage cells [51], (vi) from the elemental content of tomato juice to that of its paste differentiated by brands and packing [52].

While measured x-ray production has been compared with the ECPSSR/ECUSAR theories in some 500 publications, their assessment becomes valid when compared with comprehensive compilations of such data. The universality of K-shell ionization cross sections, when scaled with the variables of the CPSS [23,24], CPSSR[31] and later the ECPSSR [15] theories, allows for a proficient description of the vast amount of cross sections for virtually all elements bombarded by protons and light ions. As more data than referenced originally [15,22,25,30,31,37] became available, updated comparisons with the ECPSSR were made for K- and L-shell ionization [53] as well as M-shell data [54]. Residual deviations between the data and predictions of the ECPSSR have been fitted to simple polynomials to obtain semiempirical fits [55].

Comparisons with the predictions of the ECPSSR theory included compilations of data for K-shell ionization by protons and He ions [56] and L-shell ionization by protons [57]. Tables of the ECPSSR cross sections [58] and codes [59] that evolved with modifications of that theory provide for calculations of these cross sections. As noted in [41,60], these tables and codes deviate from the original ECPSSR/ECUSAR formulation. While cross sections for these tables [58] and in these codes [59] have been integrated between exact instead of approximate momentum transfers and a multiplicative correction with the energy-loss function of [15,44], the m_R factor from [31] that accounted for the relativistic effect in the ECPSSR theory was [58] and continues [59] to be incorrectly inserted in the expressions for these exact momentum transfers.

As proposed in [39], the ECPSSR theory and its modifications were tested with experimental ratios of antiproton-to-proton ionization cross sections [61]. Analytical cross sections for K-shell ionization by nonrelativistic protons were scaled to protons at relativistic velocities [62] that are relevant for high-energy PIXE and beyond for 1-GeV-protons of galactic cosmic radiation. It would be interesting to apply [62] in calculations of inner-shell ionization cross sections by, presumed constituents of dark matter, 100–300 GeV WIMPS [63].

Formulas of the ECPSSR theory are expressed in terms the plane-wave Born cross sections calculated with the screened hydrogenic wavefunctions. Based on tabulated values [64], and as evaluated numerically with Hartree Slater [65] or Dirac Hartree Slater wavefunctions [65,66], these cross sections tend to be 10–20% smaller than the ECPSSR or ECUSAR at intermediate and high proton energies for both K-shell [41] and L-shell [44,67]. In slow collisions and especially for heavy targets, with the decreasing energy the ratio of cross sections evaluated with the DHS wavefunctions to the screened hydrogenic results rises above 1 by as much as a factor of 2 for the K shell [65] and above 1 by almost the same factor of 2 for the L shell [44]. As noted in [41,42,44,67–69], the function that accounts in the ECPSSR for the perturbed stationary state (PSS) of the inner shell of a separated atom overestimates the increase binding relative to the binding energy in the united atom (UA). Cross sections due to better wavefunctions for the K shell are in part larger because the UA approach was combined with DHS wavefunctions in [65,66] albeit the UAcorrection was significant only for light target elements in slow collisions.

It is in that slow collision regime of the low-energy PIXE where the validity of the Coulomb factor proposed by Brandt et al. [14,33–35,41,44] has been challenged [70].

While better wavefunctions and the ECUSAR increase cross sections over the ECPSSR evaluated with SH wavefunctions, smaller values of the Coulomb deflection factor [70] would compensate for such an increase,

For the L shell, interpretation of L-subshell ionization is clouded by the role of intra-shell transitions [71]. According to coupled-state calculations [72], which claimed to better than the simple approximation [71], the intra-shell couplings did not significantly change L_i-subshell cross sections in ionization by protons and helium ions. Yet based on the formulas that were published afterwards [71], with the decreasing projectile energy, the intra-shell transitions boost L_2 cross sections by as much as 50% while slightly decreasing L_1 cross sections and having virtually no influence on L_3 subshell [44]. With an appropriate normalization of the formulas given in [71], the cross section for the total L-shell ionization is essentially unaffected by the intra-shell transitions [67]. A method was proposed to extract L_i subshell cross sections by least-square fitting semiempirical functions to an updated database of only $L_{\alpha+\beta}$ and L_γ ray cross sections [73].

Comparisons of x-ray production cross sections to predictions of any ionization theory hinge on the choice of atomic parameters [67,74]. Recommended sets of atomic parameters might have been derived from the data that had systematic errors [75]. The errors in both the ionization theory and the atomic parameters could conspire to cancel each other [76]. The selection of appropriate atomic parameters is especially critical for light target atoms where comparisons with an ionization theory are also affected by their multiple ionization [67,77]. Simultaneous measurement of x-ray production and Auger-electron cross sections as it was last done four decades ago [78] would segregate and directly test the effect of multiple ionization on the atomic parameters that are employed to convert ionization to x-ray production cross sections that enter in PIXE analyses. While heavy target atoms are not as critically affected by multiple ionization, more measurements across the periodic table beyond uranium to test such data – as it was done recently with the ECPSSR – has been urged in [79].

Brandt's legacy for PIXE analyses, a theory for accurate and reliable inner-shell ionization cross sections, may require theoretical fine tuning to examine a synergetic interplay of the energy-loss, Coulomb-deflection, united-atom, relativistic wavefunction, and multiple ionization effects as they all become more prominent and cancelling each other to some degree with the decreasing projectile's energy. Ultimately any theory needs to be firmly established by experiment with a renewed endeavor in measurements of x-ray production cross sections by protons and light ions. With the global proliferation of Geant4 Toolkit [80], theoretical cross sections developed after the work of Brandt – or with any other theory that can be properly scaled in universal variables to cover a wide area of projectile energies and target atoms without enormous numerical efforts – must be scrutinized by the latest and most comprehensive experimental databases [81]. A very recent compilation of L-shell x-ray production and ionization cross sections by protons [82] nearly doubles the database from the previously published tables [57].

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