Ternary ridge of ejected electrons from fast ion-atom collisions

C. O. Reinhold and D. R. Schultz
Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6373

U. Bechthold and G. Kraft
Gesellschaft für Schwerionenforschung, m.b.H., Planckstraße 1, D-64291 Darmstadt, Germany

S. Hagmann
J. R. Macdonald Laboratory, Kansas State University, Manhattan, Kansas 66506

H. Schmidt-Böcking
Institut für Kernphysik, August-Euler-Straße 6, D-60486 Frankfurt, Germany

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We present a theoretical analysis of the spectrum of swift electrons resulting from collisions of 5.9 MeV/u U^{29+} with Xe atoms. Our calculations include, within an independent model, all sources of electrons (i.e., target L-O shells and projectile O-P shells). We show that there exists clear evidence for a ternary ridge of swift electrons originating from head-on collisions between target electrons and the impinging projectile followed by elastic scattering at the target core. These findings provide a theoretical confirmation of an experimental observation of a ternary ridge in isolated ion-atom collisions. [S1050-2947(98)03009-1]

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I. INTRODUCTION

The production of swift (''hot'') electrons in ion-atom and ion-solid collisions has drawn the attention of numerous researchers during the last decade. Much of this work has been devoted to finding signatures of the so-called ''Fermi shuttle'' mechanism [1] according to which an electron can be accelerated by successive head-on collisions with a moving heavy ion (the projectile) and a heavy core nearly at rest (the target). If the velocity of the former is denoted by v_p, every head-on collision between the electron and the projectile leads to an increase of $2v_p$ in the momentum of the electron (atomic units are used throughout except where explicitly noted). Successive collisions could therefore yield hot electrons whose outgoing velocities are multiples of $2v_p$ [2]. Despite its apparent simplicity, however, distinct signatures of ionizing, multiple-scattering events from single ion-atom collisions have been very difficult to observe (e.g. [3]), the first clear result only recently being obtained [4].

Also of relevance to this search was work in the early 1990's on cluster-impact fusion (e.g., [5]), which considered the Fermi-shuttle mechanism to be a key ingredient to the proposed scheme. However, quantitative estimates of the efficiency of such a process showed that it was not feasible (e.g., [6]). The inefficiency of the Fermi-shuttle mechanism is related to the fact that for multiple collisions to occur, nearly zero impact parameter collisions are required whose contribution to the total cross section is negligible [i.e., since $\sigma = \int b\,db\,P(b)$]. Collisions involving bare projectiles were shown to be particularly inefficient for producing many hot electrons. Subsequently, various works have shown that the production of hot electrons is considerably enhanced for screened projectiles. For collisions near surfaces or in solids, a large amount of screening could be provided by the nearly free electron gas in the solid. Such a model has been recently proposed [7] to explain experimental observations of an unusually large number of hot electrons resulting from ion-surface collisions [8], which was subsequently attributed to negative ions [9]. In turn, considerable screening in binary atomic collisions can be accomplished using clothed (i.e., partially stripped) ions and targets with many occupied electronic orbitals, which leads to a pronounced enhancement of the yields of hot electrons [10–12].

Exploiting this concept and seeking signatures of multiple scattering, an experiment has been recently designed using fast, clothed uranium ions colliding with various gaseous targets [4]. Due to the large amount of screening (i.e., small value of q/Z, the ratio of the ionic charge to the nuclear charge) of the projectile, this experiment has been able to prove the existence of a ''ternary'' ridge of hot ejected electrons that is associated with a double scattering mechanism. Ternary ridges had been previously observed in ion-solid [13,14] and ion-surface [15] collisions. In these cases, however, the production of ternary electrons is greatly enhanced because the hot electrons can be rescattered by a large number of target cores in the solid. Therefore, the observation of a ternary ridge from isolated ion-atom collisions was quite surprising. Despite the sufficiently low pressure of the gas target, it has been speculated that the observed electrons might not arise from a single ion-atom collision but instead from scattering of binary electrons by other target atoms in the gas, much like in ion-solid collisions. The present brief work has been motivated by this potential controversy and we have performed a series of calculations that indeed confirm the experimental findings.

II. RESULTS AND DISCUSSION

Figure 1 displays the experimental momentum distribution of ejected electrons from 5.9 MeV/u U^{29+}-Xe collisions

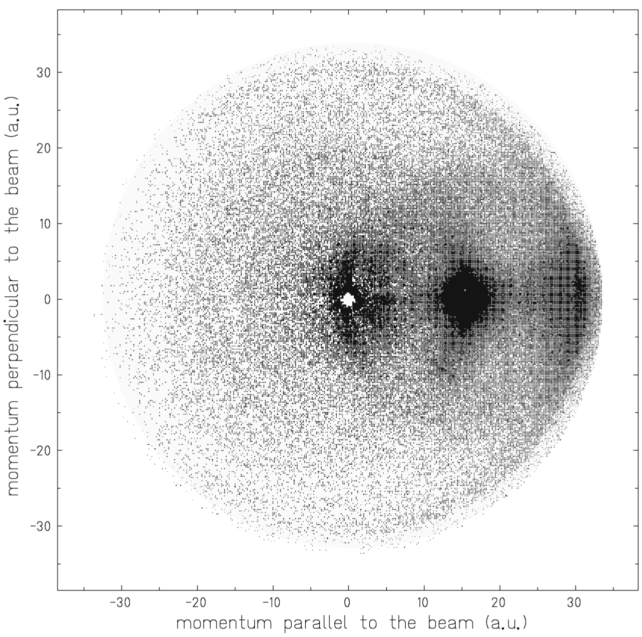

FIG. 1. Experimental momentum distribution of ejected electrons in collisions of 5.9 MeV/u U^{29+} ions with Xe. The size of points in the figure is proportional to $\ln(d^2\sigma/dpd\Omega)$, where p is the electron momentum and Ω is the emission solid angle in the laboratory frame. The abscissa indicates the value of $\vec{p}$ parallel to the projectile velocity vector, and the ordinate indicates the component perpendicular to $\vec{v_p}$. Due to the limited scanning voltage of the analyzer the spectrum is cut at velocities larger than 33 a.u. Due to efficiency problems the intensity at very small momenta is somewhat suppressed and set to zero for small momenta. The spectrum is cut for momenta $p<33$ a.u. due to the limited scanning voltage of the analyzer.

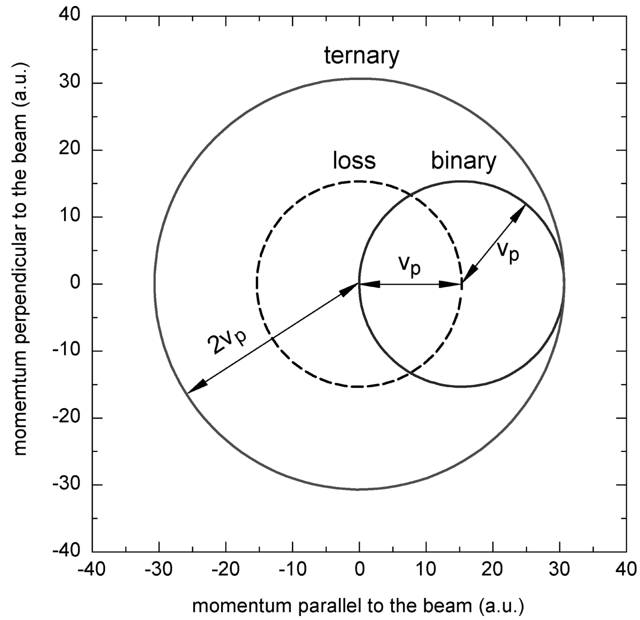

FIG. 2. Schematic diagram of possible ridges in the ejected electron momentum distribution originating from binary, ternary, and loss events for a collision energy of 5.9 MeV/u (a collision velocity $v_p = 15.3$ a.u.).

which clearly exhibits various scattering structures, a diagram of which is shown in Fig. 2 identifying the ringlike structures observed. First, a close collision between a target electron and a fast projectile usually leads to a circular ridge of electrons centered at $\vec{p}=(v_p,0)$ ($v_p=15.3$ a.u.) with a radius equal to v_p. Observations of this so-called ''binary'' ridge have existed in the literature for decades. The same structure has been observed numerous times for ionization of the projectile and is usually referred to as the ''loss'' or ''electron loss'' ridge. In this case, the ridge is centered at $\vec{p}=(0,0)$.

For considerably screened ions (i.e., ions with small q/Z), the binary ridge exhibits a dramatic enhancement in intensity at zero emission angle or $\vec{p}\simeq(2v_p,0)$ (see Fig. 1). These electrons originate in head-on (nearly zero impact parameter) collisions with the projectile. Within the present context, the most important consequence of the enhancement due to screening is that it provides an intense and well defined source of electrons for re-scattering by the target core. Indeed, if these electrons are subsequently scattered by the target field, they end up in a circular ridge centered at $\vec{p}=(0,0)$ with a radius of $2v_p=30.6$ a.u. Such a ''ternary'' ridge is evident in Fig. 1 and constitutes a clear signature of double scattering. In the following, we present a theoretical analysis of this experimental spectrum.

Our analysis employs a well established approach in ion-atom collisions: the classical trajectory Monte Carlo (CTMC) method [16–18]. A calculation of the ejected electron spectrum in fast collisions of U^{29+} with Xe atoms is quite complex because of the large number of electrons that become involved. Inner shells cannot be ignored because of the large average momenta of electrons in these orbitals, which plays a very important role in the emission of hot electrons. In addition, any realistic calculation must incorporate the distance-dependent screening of the projectile and target cores and should account for two-center effects (the simultaneous interaction of the electrons with the target and the projectile). Here we consider all of the electrons in the $n=2,3,4,5$ shells of Xe and the $n=4,5,6$ shells of U^{29+} within an independent-electron approximation (electrons interact with each other only through static screening potentials). Each electron is initially bound to the target or the projectile core by an energy equal to the Hartree-Fock orbital energy and interacts with both heavy centers through model potentials, which yield the correct Hartree-Fock orbital energies of the ions [19].

Hot electrons are usually the result of a large momentum transfer delivered to the electrons and are well described by classical dynamics [20]. Screened ionic cores, however, may lead to departures from classical dynamics when the de Broglie wavelength of the electron becomes comparable to the screening length of the cores. This leads to diffraction oscillations, which are well documented in the literature [21–25]. Fortunately, as shown in Fig. 3, a collision energy of 5.9 MeV/u ($v_p=15.3$ a.u.) is large enough that the classical and quantum differential cross sections for elastic scattering of electrons by the ionic cores considered here are in reasonable agreement. In particular, for the target ion, Xe^+, the classical and quantal results nearly coincide. The most severe disagreement is found at backward angles for scattering at U^{29+}, which corresponds to forward angles in the laboratory frame (projectile, θ, and laboratory, θ_L, scattering angles are

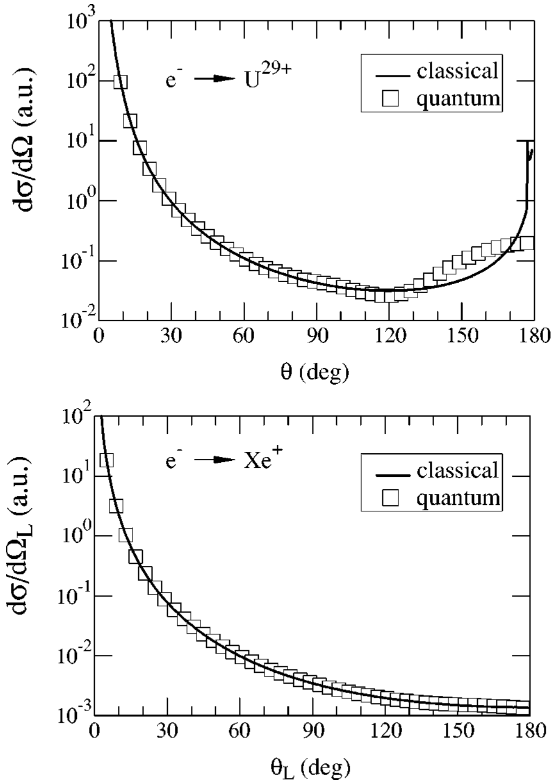

FIG. 3. Classical (dashed line) and quantum (solid line) differential cross sections for elastic scattering of an electron with a velocity of 15.3 a.u. (30.6 a.u.) by a U^{29+} (Xe^{+}) ion, representing the initial encounter of the electron with the projectile, and, once scattered into the forward direction at $2\,v_p$, with the target core. Both calculations are ''exact'' within the framework of potential scattering and we use the static model interactions of Ref. [19]. The quantum results have been obtained using a standard partial wave expansion and numerically solving the corresponding radial Schrödinger equation.

related by $\cos\theta = 1 - 2\cos^2\theta_L$). The classical cross section at $\theta \sim 180°$ exhibits the usual rainbow and glory divergences whose quantum analog is an enhancement of the backward cross section. This enhancement is a direct consequence of screening and is responsible for the very intense ''source'' of forward binary electrons in Fig. 1. Note, however, that the half angular width of the forward ''source'' of $\vec{p} = \sim(2v_p,0)$ electrons is about $\sim 10°$, which translates to a half angular width of $\sim 20°$ in the projectile frame. The average of the classical and quantum cross sections over a solid angle in this range agree with each other within a factor of 1.5. Therefore, a classical calculation at this high collision energy is expected to yield reasonable results.

Figure 4 displays the calculated momentum distribution of ejected electrons corresponding to the experimental data in Fig. 1. The calculations exhibit clear signatures of the binary and ternary ridges, much like in the experimental data. However, the calculated ternary ridge is less pronounced than the experimental one. At an emission angle of 45° the experimental intensity of ejected electrons is clearly separated into the binary and ternary peaks. In turn, the calculated intensity exhibits a shoulder in the region of the ternary ridge (i.e., the intensity is nearly flat up to $p \sim 2v_p$, around where it drops dramatically). Inner shells of Xe con-

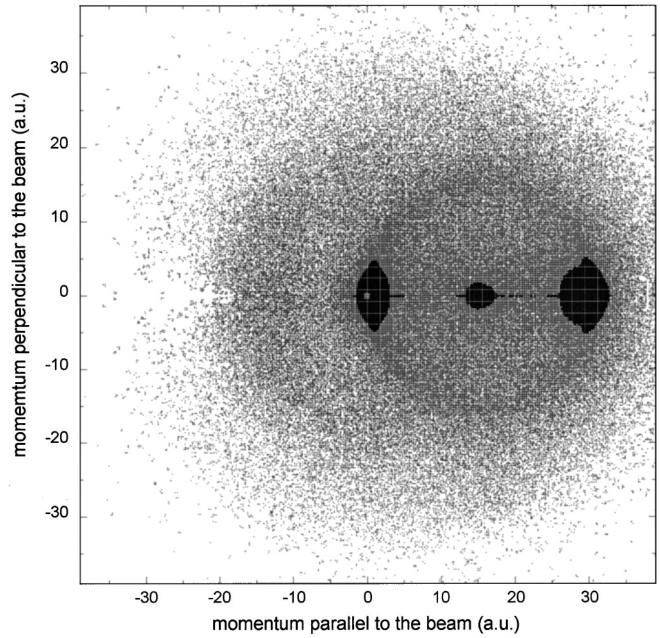

FIG. 4. Calculated scatter plot of the momentum distribution of ejected electrons, $\ln(d^2\sigma/dpd\Omega)$, corresponding to the experimental spectrum in Fig. 1.

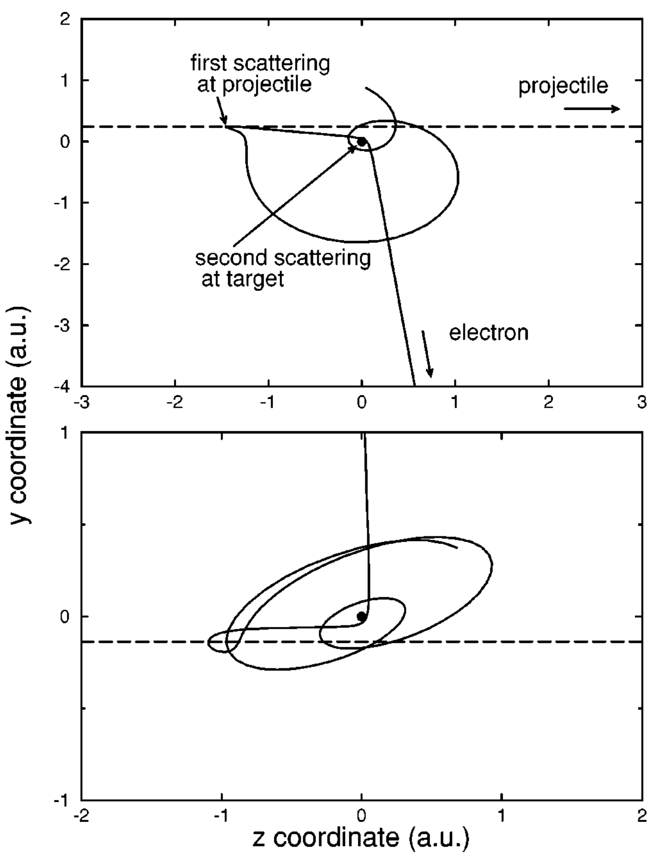

FIG. 5. Typical trajectories leading to hot electrons in the neighborhood of the ternary ridge. The solid line represents the electron, the solid circle is the target core and the dashed line correspond to the projectile which moves towards infinity on the positive z axis. The final velocity of the electron is similar to $2v_p$.

tribute significantly to the ternary ridge and their broad Compton profiles are actually responsible for its lack of sharpness (a sharper ridge is obtained if only the valence shell of Xe is considered in the calculations). Remarkably, ionization (stripping) of U^{29+} also plays a role in the ejected electron spectrum and gives rise to a diffuse but visible loss ridge.

In order to verify the actual origin of electrons in the region of the ternary ridge, we have followed the evolution of several relevant electron trajectories. Figure 5 displays two typical trajectories in the y-z plane, where the projectile moves towards the positive z axis. The electron, initially in an orbit about the target core, is attracted towards the impinging projectile, scatters violently with such a deflection angle that it is directed towards the target core, where it suffers another collision. We find that, indeed, the majority of $|\vec{p}|\sim 2v_p$ electrons emitted at large angles originate in a nearly head-on collision with the projectile followed by scattering by the recoil target ion. Evidently, for this to occur, the z coordinate of the electron must be less than that of the target core $(z=0)$ at the moment that the electron collides with the projectile.

Summarizing, we have performed a complete and realistic calculation of the ejected electron spectrum from fast U^{29+}-Xe collisions. The results of our simulation confirm the recent experimental observation of a ternary ridge in isolated ion-atom collisions.

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