Inner-shell excitation in heavy-ion–solid-target collisions

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In this Rapid Communication an *ab initio* approach to the inner-shell charge-transfer process in heavy-ion–solid-target collisions is presented. Unlike the extensively studied ion–gas-target systems heavy-ion–solid-target measurements showed systematic deviations from available theories. These deviations were interpreted as revealing a fundamental difference between collisions with gas and those with solid targets. Within the framework of our relativistic formalism a quantitative description of heavy-ion–solid-target charge-transfer processes is reached, thus laying to rest the old problem of solid-target effects. As an example, the results for Cu on a Ni solid target are discussed.

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From a theoretical point of view inner-shell processes in adiabatic ion–solid-target collisions involving heavy collision partners ($Z_{T,P} \geqslant 20$) are not yet well understood. A whole series of experimental papers dealing with ion–solid-target collisions has been published over the last two decades (as an example see Refs. [1–3] and Ref. [4], and references therein). The object of most of these papers was to provide an insight into the target thickness dependence of the *K-L* vacancy transfer probabilities. Studying the target thickness was thought to be important first in terms of whether or not multiple *K-L* vacancy transfer processes take place, and second, in the case of projectiles that do not have any initial *L* vacancies, to understand how *L* vacancies are created dynamically and then transferred to the *K* shells.

A qualitative interpretation of most of the experimental results was given within the framework of the $2p\pi$-$2p\sigma$ Briggs-Taulbjerg coupling scheme [5,6]. At most the $2p\pi$-$2p\sigma$ scaling gives an approximate qualitative description of the $P(b)$ curve but fails on the quantitative explanation and the reproduction of the location of maxima and minima. These discrepancies between the $2p\pi$-$2p\sigma$ scaling law and experimental results, especially in the adiabatic region, were thought to reveal a fundamental difference between ion–gas- and ion–solid-target collision systems. Based on this assumption ongoing fundamental experiments looking at the adiabatic inner-shell charge transfer in slow collisions of nearly naked super heavy ions with atoms were proposed by Ulrich to be done with gas targets instead of solid targets [7]. Using the latter target type would dramatically reduce the costs, raise the efficiency, and speed this type of experiment.

Ab initio full scale calculations, especially for heavy systems where both the relativistic effects and the many-particle aspect are important, are not yet available for heavy-ion–solid-target collision processes: An early six-channel relativistic close-coupling calculation performed by Heiligenthal *et al.* [8] for the super-heavy system U-Pb focused exclusively on the kinematic peak region. de Reus *et al.* [9] performed relativistic adiabatic time-dependent Hartree-Fock calculations for the direct inner-shell excitation and electron-positron pair creation in super-heavy near symmetric systems.

Using our *ab initio* relativistic time-dependent Dirac-Fock-Slater method we demonstrate that the experimental results for the impact-parameter-dependent charge-transfer probability can be explained both qualitatively and quantitatively. It has become obvious that beside the importance of both the radial and rotational coupling in the *K-L* charge-transfer process, additionally the dynamic many-particle aspect of the collision system has to be taken fully into account.

The time-dependent Dirac-Fock-Slater basis-set method used by us can be read up on in a series of papers [10–12] and references therein. The paper of Sepp *et al.* [10] presents in detail the generation of relativistic basis functions, while the papers of Kürpick *et al.* [11,12] describe the calculation of *ab initio* dynamic coupling matrix elements used in the close-coupling equation

$$\dot{a}_{ij} = \sum_j -a_{im} \left\langle \phi_j \left| \dot{R} \frac{\partial}{\partial R} - \frac{i\dot{\theta}}{\hbar} j_y^{\mathrm{CM}} \right| \phi_m \right\rangle \times \exp\left(-\frac{i}{\hbar} \int (\varepsilon_m - \varepsilon_j) dt' \right)$$

and the application of the method to heavy-ion-atom collisions involving gas targets. For the definition of the variables, we would like to refer to Refs. [11,12]. As in this Rapid Communication we solely focus on adiabatic heavy-ion collision systems with $Z_{\mathrm{united}} \leqslant 40-60$, direct ionization is of no importance and there is no need to take continuum states into account.

We have calculated a number of systems that all yield the same very good agreement with experimental results. In this Rapid Communication we present as an example results for Cu on Ni where detailed measurements from Annett *et al.* [1] are available. To obtain an adequate description of the Cu-Ni collision system, which will serve as an example of the influence of dynamics in the *K-L* vacancy transfer in ion–solid-target collisions, we use 28 molecular four-component–Dirac-Fock-Slater basis functions generated by solving the static Dirac-Fock-Slater equation at about 100 internuclear distances ranging from 0.005 to 10 a.u. As seen in the correlation diagram in Fig. 1 this allows us to take the

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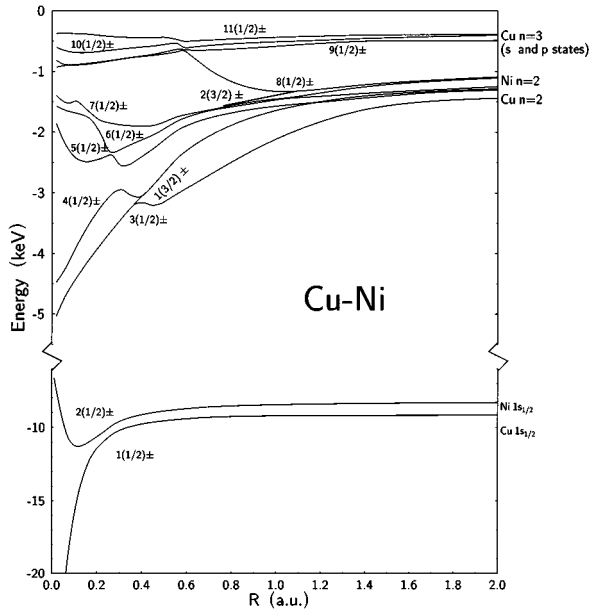

FIG. 1. Correlation diagram for the system Cu-Ni. The molecular $1(1/2)\pm$ and $2(1/2)\pm$ levels correspond asymptotically to the Cu $1s_{1/2}$ and Ni $1s_{1/2}$ atomic states.

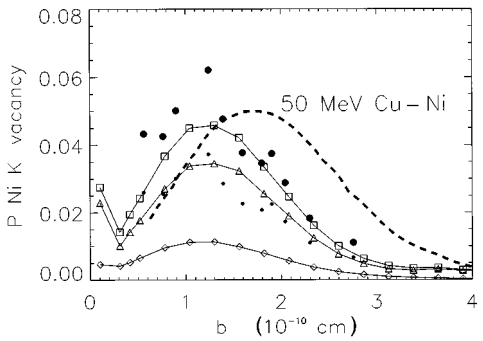

FIG. 2. $P_{\text{Ni-}K}$ vacancy probability for 50-MeV impact energy: The large black circles show the experimental results for the Ni K vacancy production probability of Annett *et al.* [1] obtained with the 6-μg/cm^2 target. The triangles show the weighted contribution of the M shell holes to the Ni K vacancy production probability. The diamonds show the weighted contribution of the L-shell holes to the Ni K vacancy probability. The squares show the total Ni K vacancy probability as the sum of the former two probabilities. The small black circles show the experimental low target thickness results for the Ni K x-ray production probability scaled from the former experimental results according to the target thickness dependence measured by Annett *et al.* [1]. The broken curve shows the scaled theoretical results for the $2p\pi$-$2p\sigma$ rotational coupling model of Taulbjerg, Briggs, and Vaaben [6].

Cu $n=1$, $n=2$, $n=3$ (s and p states) and Ni $n=1$, $n=2$ shells into account. As a test of the convergence of the employed basis we increased it up to 40 channels, but no significant change in the impact-parameter-dependent probabilities discussed below was observed.

Apart from providing the impact-parameter-dependent Ni K vacancy production probability (shown in Fig. 2 as large black circles) the measurements of Annett *et al.* also resolved the final charge state of the Cu projectile. For 50-MeV impact energy they displayed a 87% probability of lying between $q=16$ and $q=20$. This result is not surprising, as the $n=3$ Cu states do not behave adiabatically at 50-MeV impact energy and are furthermore easily ionized in a thin target [12].

As a first step we evaluate the coupling between the Cu $n=2$ and the Ni K shell by performing close-coupling calculations in the subspace of the molecular $1(1/2)\pm$ to $5(1/2)\pm$ and $1(3/2)\pm$ states. The coupling from the higher states to the $2(1/2)\pm$ state, which correlates to the Ni K shell, turned out to be quite strong. The probability of a vacancy being transferred from the $1(3/2)\pm$ to the $2(1/2)\pm$ state while permitting no coupling to higher channels is as high as 15%. Similar results are obtained for the $3(1/2)\pm$ and $4(1/2)\pm$ states. Therefore, the coupling from the Cu $n=2$ shell to the Ni K shell is quite strong.

Keeping this in mind, we performed close-coupling calculations for two different charge states of the Cu projectile, using the full basis set of 28 molecular channels. Our first full scale calculation used a Cu^{19+} projectile, i.e., only M vacancies were initially available. We therefore took all electrons of the Cu and Ni $n=2$ shell into account and permitted them to couple with each other as well as with the empty Cu $n=3$ shell. These many-particle calculations, with a completely empty Cu M shell and full K and L shells, reveal a strongly damped Ni K vacancy probability with a maximum of about 5% at $b=2500$ fm caused by dynamic creation and annhilation of vacancies among the Cu $n=2$, $n=3$ and Ni $n=2$ shells. A time-dependent analysis of the channels verifies both a promotion of the initial Cu $n=2$ shell electrons to the empty Cu $n=3$ shell and a partial refilling of the Cu $n=2$ shell by Ni $n=2$ electrons; the result is a smaller effective Cu L-vacancy rate.

In a second step we performed calculations using Cu^{20+} as a projectile, which allows the Cu projectile to have one initial vacancy in the L shell. The corresponding Ni K vacancy probability $P(b)$ almost doubles to about 10% at the maximum, the shape of the $P(b)$ curve being almost the same.

In order to compare our theoretical K-L vacancy transfer probability to the Ni K x-ray production probability, measured by Annett *et al.* for the 50-MeV Cu-Ni collision system, we now proceed as follows: We weight the mean Ni K vacancy probability (which we obtained for the Cu^{19+} projectile with no initial Cu L vacancy but an empty M shell) with the charge-state fraction of M vacancies of the projectile in the final state, as shown in Table 1 in the paper of Annett *et al.* [1]. Figure 3 shows these weighted $P(b)$ curves as triangles. It provides the partial Ni K vacancy probability for all projectiles with a charge state up to $q=19+$.

Using the Ni K vacancy probability obtained by us for Cu^{20+} we proceed in the same manner as before and calculate the weighted Ni K vacancy probability for all projectiles with a charge greater than $q=19+$. Figure 3 shows the resulting partial Ni K vacancy probability as diamonds.

The total Ni K vacancy probability (drawn as squares in Fig. 2) is given as the sum of both partial probabilities. It compares very well with the experimental curve for the 6-μg/cm^2 target corrected for the fluorescence yield.

Additionally, we plotted the result obtained with the

$2p\pi$-$2p\sigma$ rotational coupling theory from Taulbjerg, Briggs, and Vaaben [6] as a broken curve. This later result was normalized to reach the height of the experimental values and shows a large shift of the maximum towards higher impact parameter.

These results clearly favor the interpretation that at very small target thicknesses (up to a few monolayers) only M-shell vacancies are generated in a stationary way. Indeed, our results for the partial M-shell vacancy contribution to the Ni K vacancy production compare very well with the experimental Ni K vacancy production curve scaled to the low target thickness limit by using the measured target thickness dependence of Annett *et al.* [1]. These scaled experimental results are shown in Fig. 2 as small black circles.

In this Rapid Communication we have presented *ab initio* relativistic calculations on the K-L vacancy transfer in heavy-ion–solid-target collisions. Our method provides not only a very good qualitative and quantitative agreement and understanding of experimental results but also disproves the old assumption that additional solid-target effects are responsible for the discrepancy between the results from the $2p\pi$-$2p\sigma$ rotational coupling scheme and experimental $P(b)$ curves. Preliminary results for the Ni-Ge solid-target collision system [13] also exhibit an excellent agreement with recent measurements of Jäger *et al.* [14].

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