ELSEVIER

30 October 1995

PHYSICS LETTERS A

Physics Letters A 207 (1995) 199–202

Full scale relativistic ab initio time dependent calculations for the L–K vacancy transfer in 208 MeV Ni^{23+} on a Ge solid target

P. Kürpick [a,1], T. Baştuğ [a], B. Fricke [a], W.-D. Sepp [a], A. Warczak [b], M. Jäger [c], J. Ullrich [c], T. Kandler [c], M. Schulz [d], A. Demian [e], M. Damrau [e], H. Bräuning [e], H. Schmidt-Böcking [e]

[a] *Fachbereich Physik, Universität Kassel, 34109 Kassel, Germany*
[b] *Department of Physics, University of Cracow, Cracow, Poland*
[c] *Gesellschaft für Schwerionenforschung (GSI), 64220 Darmstadt, Germany*
[d] *Department of Physics, University of Missouri, Rolla, MO, USA*
[e] *Institut für Kernphysik, Universität Frankfurt, Frankfurt, Germany*

Received 30 May 1995; revised manuscript received 4 September 1995; accepted for publication 5 September 1995
Communicated by P.R. Holland

Abstract

We present full scale ab initio relativistic calculations for the L–K vacancy transfer in collisions of 208 MeV Ni^{23+} on a Ge solid target. Our Dirac–Fock–Slater method allows us to achieve a very accurate quantitative explanation for the experimental impact parameter-dependent vacancy probabilities in terms of dynamic creation and annihilation of Ni $n = 2$ shell vacancies.

PACS: 34.10.+K

Since the late seventies a whole series of experimental investigations on the inner shell vacancy transfer in collisions of heavy ions with solid targets has been performed [1–8]. The aim of these experimental projects was to understand both the charge state distribution of the projectile while it travels through the solid target and the dynamic creation of M- and L-shell vacancies and their further transfer to the K-shell. A more complex behaviour was expected in ion–solid target collisions as compared to ion–gas target collisions as it was not clear which behaviour the projectile would show while traveling through the periodic lattice of the solid target.

From a theoretical point of view ab initio calculations for ion–solid target collisions including both the relativistic effects of the electrons of the collision system in the framework of a Dirac–Fock approach and its many particle aspect were not available up to now. The interpretation of most of the experimental results was done in the framework of the nonrelativistic $2p\pi$–$2p\sigma$ coupling scheme as proposed by Briggs and Taulbjerg [9,10]. On the other hand Anholt, Meyerhof and Salin [11] as early as in 1977 suggested that relativistic effects, which should be significant in heavy ion collisions, could lead to a discrepancy to the nonrelativistic $2p\pi$–$2p\sigma$ coupling results. In particular they predicted an increase of the K-vacancy probability for small impact parameters.

Using our ab initio time dependent relativistic

[1] Present address: Department of Physics, Kansas State University, Manhattan, KS 66502, USA

SSDI 0375-9601(95)00681-8

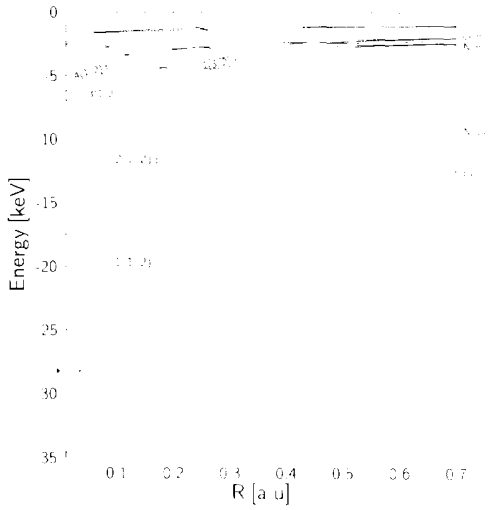

Fig. 1. Correlation diagram for the system Ni^{23+}–Ge. The molecular $1(1/2)\pm$ and $2(1/2)\pm$ levels correspond asymptotically to the Ge $1s_{1/2}$ and Ni $1s_{1/2}$ atomic states.

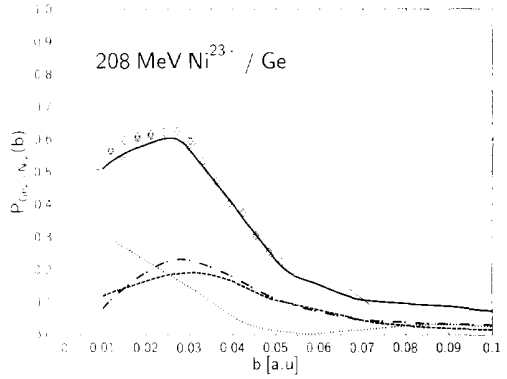

Fig. 2. Sum of the Ge–K and Ni–K vacancy probabilities. Experimental values: diamonds: 11.5 $\mu g/cm^2$ target; circles: 5.0 $\mu g/cm^2$ target; thin curve: nonrelativistic normalised $2p\pi$–$2p\sigma$ coupling result [10]; thick curve: our result for the sum of the probabilities to have at least one vacancy in the molecular $1(1/2)\pm$ level resp. $2(1/2)\pm$ level; broken curve: partial contribution from the initial $3(1/2)\pm$ vacancies; dotted curve: partial contribution from the initial $4(1/2)\pm$ vacancies; chained curve: partial contribution from the initial $1(3/2)\pm$ vacancies.

Dirac–Fock–Slater method we took up this old problem and present an explanation for both the dynamic L-shell vacancy creation and their later transfer to the K-shells of the collision partners.

This method and its application to ion–gas target systems has been described in detail in Refs. [12–14]. The numerical solution of the stationary two-center-Dirac–Fock–Slater equation by means of the LCAO-MO method was presented in an early paper of Sepp et al. [12] while the evaluation of dynamic radial and rotational coupling matrix elements can be found in a recent paper of Kürpick et al. [14].

To get a complete basis set and therefore an accurate description of the present Ni^{23+}–Ge system we span the Hilbert space using numerically given $1s_{1/2}$ to $3p_{3/2}$ atomic orbitals on the Ni-site and $1s_{1/2}$ to $4s_{1/2}$ atomic orbitals on the Ge-site. These wave functions enter as a basis for the solution of the stationary two center Dirac–Fock–Slater equation, which is then solved at 100 internuclear distances ranging from 0.001 to 10 a.u. Fig. 1 shows the resulting correlation diagram for the lowest 24 molecular states. While the molecular $1(1/2)\pm$ and $2(1/2)\pm$ states correlate asymptotically to the Ge $1s_{1/2}$ and Ni $1s_{1/2}$ states respectively, the Ni $n = 2$ and Ge $n = 2$ shell are already energetically swapped because of the high degree of ionisation of the Ni projectile.

The actual time dependent close coupling calculations are then performed in the subspace of these 26 molecular orbitals $1(1/2)\pm$ to $10(1/2)\pm$ and $1(3/2)\pm$ to $3(3/2)\pm$ which is large enough to accurately describe the promotion of inner shell electrons to higher shells.

In the first step we studied the large impact parameter range from 0.1 up to 2.0 a.u., which is quite common for a projectile which travels through a solid target. Our assumption was that the Ge $n = 2$ electrons are partially promoted to higher shells but also produce a dynamic occupation of the initially almost empty Ni $n = 2$ shell, which has three electrons and five vacancies in the incoming channel. Indeed we observe this phenomenon in our close coupling calculations. They reveal a 50% filling of the Ni $n = 2$ shell therefore leading to approximately four vacancies in the Ni $n = 2$ shell in the dynamical equilibrium. As we work with a finite basis set these calculations can only give an approximate picture of the mean charge state of the projectile. Nevertheless, it can be derived that the mean charge state of the Ni-projectile, while traveling through the target and repeating large impact parameter collisions with neutral Ge-atoms, should be about $q = 23-$, which is verified experimentally [15,16].

Former experimental results, as performed for example by Annett et al. [4] on the system Cu^{9+} on Ni, had shown that for initially low charged projectiles a strong dependence of the absolute height of the $P(b)$-curves on the target thickness was observed. The present UNILAC-experiment [8] was performed using Ni^{23+} on Ge, therefore having an initial projectile charge state which is near to the equilibrium charge state of $q = 22+$ derived from our calculations. One would therefore not expect a dependence on the target thickness. Indeed the experimental impact parameter dependent Ni–K vacancy probability, presented in Fig. 2 for a target thickness of 11.5 and 5.0 $\mu g/cm^2$, shows almost no dependence on this parameter.

In the second step we investigated the rare events of a small impact parameter collision range between 0.01 and 0.1 a.u. using as initial charge state the former estimated mean number of dynamically created Ni–L vacancies at large impact parameters. The probability to have at least one vacancy in the outgoing channel was calculated both for the Ni–K and Ge–K shell. The impact parameter dependent sum of both vacancy probabilities as obtained by our method is shown in Fig. 2 as a thick curve and compared to the experimental results measured for the two target thicknesses 5 $\mu g/cm^2$ and 11.5 $\mu g/cm^2$ where the ion beam hit the target at 45 degrees to the normal incidence. The agreement with the experimental results is very good.

We have also drawn the partial contributions of the $3(1/2)\pm$, $4(1/2)\pm$ and $1(3/2)\pm$ vacancies to the $2(1/2)\pm$ and $1(1/2)\pm$ molecular levels. Besides the contribution of the $1(3/2)\pm$ vacancies, which are primarily transferred to the $2(1/2)\pm$ level via rotational coupling, one also sees the dominant role of the $4(1/2)\pm$ vacancies, especially at small impact parameters, which couple to the $2(1/2)\pm$ and $1(1/2)\pm$ molecular levels both by radial and rotational coupling. Almost 50% of the transferred vacancies come from pure radial coupling, keeping in mind that it is difficult to properly extract this quantity from our calculations.

The thin curve was evaluated within the nonrelativistic $2p\pi$–$2p\sigma$ scaling law [10]. This curve, normalised to the experimental maximum, clearly has its maximum at larger impact parameters.

Our result favours the following picture for the description of ion–solid target collisions:

First, as one proceeds to heavier projectiles and targets one clearly has to take into account the relativistic effects in the eigenvalues and in the positions of the maxima of the coupling matrix elements, which changes the shape and shifts the $P(b)$-curves.

Second, one should note that besides the rotational coupling the radial coupling also contributes drastically to the L–K vacancy transfer as can be seen from our results.

Finally, one has to keep in mind that the charge state of the projectile in an ion–solid target collision is not well defined. The ion performs multiple collisions at large impact parameters before a collision at small impact parameters occurs. Annett et al. [4] have already experimentally shown that these multiple collisions lead to a wide range of charge states of the projectile. An approximate value for the mean charge state can be obtained in our close coupling calculation. One then has to use this distribution of charge states, or at least the mean charge state, to calculate an accurate inner shell vacancy production probability.

As a concluding remark one should say that a crucial test of our proposed mechanism would be provided by experimental results both on a heavy ion–gas and a heavy ion–solid target system involving the same collision partners. An experiment undertaking these measurements is planned at GSI [17].

Support from the Deutsche Forschungsgemeinschaft (DFG) for P.K. and T.B. is gratefully acknowledged.

References

[1] B.M. Johnson, K.W. Jones, W. Brandt, F.C. Jundt, G. Guillaume and T.H. Kruse, Phys. Rev. A 19 (1977) 81.
[2] I. Tserruya, H. Schmidt-Böcking and R. Schuch, Phys. Rev. A 18 (1978) 2482.
[3] R. Schuch and G. Nolte, Z. Phys. A 293 (1979) 91.
[4] C.H. Annett, B. Curnutte and C.L. Cocke, Phys. Rev. A 19 (1979) 1038.
[5] R. Schuch, G. Nolte and H. Schmidt-Böcking, Phys. Rev. A 22 (1980) 1447.
[6] R. Schuch, R. Hoffmann, K. Müller, E. Pflanz, H. Schmidt-Böcking and H.J. Specht, Z. Phys. A 316 (1984) 5.
[7] T. Kambara, R. Schuch, Y. Awaya, T. Mizogawa, H. Kumagai, Y. Kanai, H. Shibata and K. Shima, Z. Phys. D 22 (1992) 451.
[8] M. Jäger, M. Schulz, T. Kandler, A. Warczak, H. Bräuning, A. Demian, M. Damrau, A. El-Sadek, K. Freitag, J. Ullrich and H. Schmidt-Böcking, Nucl. Instrum. Meth. B 98 (1995) 488.

[9] U. Fano and W. Lichten, Phys. Rev. Lett. 14 (1965) 627.
[10] K. Taulbjerg and J.S. Briggs, J. Phys. B 8 (1975) 1895; K. Taulbjerg, J.S. Briggs and J. Vaaben, J. Phys. B. 9 (1976) 1351.
[11] R. Anholt, W. Meyerhof and A. Salin, Phys. Rev. A 16 (1977) 951.
[12] W.-D. Sepp, D. Kolb, W. Sengler, H. Hartung and B. Fricke, Phys. Rev. A 33 (1986) 3679.
[13] P. Kürpick, H.-J. Lüdde, W.-D. Sepp and B. Fricke, Z. Phys. D 22 (1992) 451.
[14] P. Kürpick, W.-D. Sepp and B. Fricke, Phys. Rev. A 51 (1995), in press.
[15] K. Shima et al., At. Data Nucl. Data Tables 51 (1992) 173–241.
[16] P.H. Mokler et al., Nucl. Instrum. Methods B 83 (1993) 37.
[17] J. Ullrich, private communication.