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Experimental K-vacancy production probabilities of nearly symmetric heavy-ion collision systems in comparison with the $2p\pi$-$2p\sigma$ rotational-coupling model

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Measurements are reported for the impact parameter (b) dependence of K-vacancy production probabilities [$P_K(b)$] in collisions of 54.4- and 90-MeV Ni with targets of Ni, Ge, and Rb. The shape of $P_K(b)$ is found to be qualitatively similar to that expected for the $2p\pi$-$2p\sigma$ rotational-coupling mechanism, but the maximum found at large b is shifted to smaller b in comparison with the predicted adiabatic maximum. This behavior is investigated systematically by applying a simple scaling law within the $2p\pi$-$2p\sigma$ rotational-coupling model on these and all published $P_K(b)$ data of nearly symmetric collision systems.

I. INTRODUCTION

The mechanism which is commonly accepted to be responsible for K-vacancy production in slow, nearly symmetric ion-atom collisions is $2p\pi$-$2p\sigma$ rotational coupling.[1] In this model an initial vacancy in the $2p\pi$ molecular orbital (MO) can be transferred by a Coriolis coupling to the $2p\sigma$ MO. Vacancy sharing[2] between the $2p\sigma$ and $1s\sigma$ MO's on the outgoing part of the collision distributes the vacancy between the K shells of the two collision partners. The sum (P_K) of the K-vacancy production probabilities for heavier and lighter collision partners P_K^H and P_K^L, respectively, can be taken, therefore, as the $2p\sigma$ excitation probability.

The theory of $2p\pi$-$2p\sigma$ rotational coupling predicts a distinct dependence of the $2p\sigma$ excitation probability ($P_{\rm rot}$) on the impact parameter b. At small b, corresponding to a center-of-mass scattering angle of 90°, a kinematic peak appears, while at large b an adiabatic peak is predicted.[1] This characteristic dependence of $P_{\rm rot}(b)$ on b can be used to test the validity of the $2p\pi$-$2p\sigma$ rotational-coupling model for describing the K-vacancy production process in nearly symmetric heavy-ion collisions. The scaling law of Taulbjerg *et al.*,[3] enables one to compare any measured $P_K(b)$ normalized to one initial $2p\pi_x$ vacancy with the prediction of $2p\pi$-$2p\sigma$ rotational coupling $P_{\rm rot}(b)$. A fair agreement between measured $P_K(b)$ and $P_{\rm rot}(b)$ was obtained previously for light collision systems ($Z_1 \simeq Z_2 \leq 20$).[4-6] For heavier collision systems ($Z_1 \simeq Z_2 \geq 25$), strong deviations of $P_{\rm rot}(b)$ from $P_K(b)$ in the position of the adiabatic peak were reported recently.[7-10] The reason for these deviations from the scaling law is still a subject of investigation.

Since Taulbjerg *et al.*[3] calculate $P_{\rm rot}(b)$ for Coulomb trajectories, their scaling law is in two parameters (b and v), and therefore does not yield a universal presentation of all $P_K(b)$ data. By assuming a straight-line trajectory (which should be a good approximation for the cases discussed in this paper) a one-parameter scaling law can be derived[1,3] within the $2p\pi$-$2p\sigma$ rotational-coupling model. This scaling law, which will be described in Sec. II, yields a universal dependence of $P_{\rm rot}$ on a reduced impact parameter b', and it should place all $P_K(b')$ data measured in the region of the adiabatic peak on a common curve.

Such a plot for the existing low-Z data ($Z_1 \simeq Z_2 < 20$)[4-6] is presented in Sec. II of the paper, and is found to form a common curve which is in good agreement with the universal curve expected theoretically. In Sec. III we describe the experimental setup used to obtain new data for the Ni on Ni, Ge, and Rb systems. In Sec. IV a universal plot of these and earlier, higher-Z ($Z_1 \simeq Z_2 \gtrsim 25$) data[7-10] are presented and deviations from theory are discussed.

II. SCALING LAW IN $2p\pi$-$2p\sigma$ ROTATIONAL COUPLING

The rotational coupling between $2p\pi$ and $2p\sigma$ MO's is treated with coupled differential equations[1] for the vacancy population amplitudes $a_{2p\sigma}$ and $a_{2p\pi}$. Following Taulbjerg *et al.*,[3] these coupled differential equations can be written in a unified form (independent of the collision system) with the following assumptions[1,3]:

Straight-line trajectory $\sin\theta = b/R$, where R is the internuclear distance and θ is the angle between internuclear axis and initial momentum vector.

$2p\pi$-$2p\sigma$ energy splitting is proportional to R^2,

$$\Delta E_{2p\pi - 2p\sigma} = \frac{1}{40} Z_A Z_B (Z_A + Z_B)^2 R^2 = \alpha(Z_1, Z_2) R^2 \quad (1)$$

[because of screening it is $(Z_A, Z_B) = (Z_1 - 1, Z_2 - 1)$].

Rotational-coupling matrix element $f(R) \equiv 1$.

Using $\theta = bv/R^2$, the coupled differential equations can be written in the form[1,3]

$$\frac{da_{2p\sigma}}{d\theta} = a_{2p\pi} \exp\left(-\frac{i\alpha b^3}{\hbar v} \int_0^\theta \frac{d\theta'}{\sin^4\theta'}\right),$$
$$\frac{da_{2p\pi}}{d\theta} = -a_{2p\sigma} \exp\left(\frac{i\alpha b^3}{\hbar v} \int_0^\theta \frac{d\theta'}{\sin^4\theta'}\right). \quad (2)$$

With respect to the reduced impact parameter $b' = [\alpha(Z_1, Z_2)/\hbar v]^{1/3} b$, these equations are independent of the collision system and their solution is a universal function $P_{\rm rot}(b')$ which represents the adiabatic peak.

This scaling law is tested in Fig. 1 where all available $P_K(b)$ data of $Z_1 \simeq Z_2 \lesssim 20$ (Refs. 4–6) which show some indication of an adiabatic peak are plotted versus b'. In order to justify the assumption of a straight-line trajectory, only data in the region of the adiabatic peak have been plotted. The largest scattering angle considered was 8°, for the case of Ne on Ne. The absolute height of the data were normalized to have approximately the same maximum value as the theoretical universal curve.

The $P_K(b)$ data of all collision systems fall within the experimental error bars on a common curve. Note that also the scaling with the projectile velocity ($b' \sim b/v^{1/3}$) is fulfilled, as can be seen from the data of 15- and 30-MeV Cl on Ar.[5] The universal curve found by solving the coupled differential equations (2) is represented by the full line. Although there are some deviations which can be explained by the simplifying assumptions made above, the agreement with this universal curve is good.

The deviations between experiment and universal curve below the maximum are due to the influence of the Coulomb trajectory and a contribution of direct $2p\sigma$ excitation.[4,6] Using a Coulomb trajectory instead of a straight line, $P_{\rm rot}(b)$ would increase below the maximum.[3] The small but systematic deviations above the maximum may be due to the inadequacy of the assumption that $f(R) = 1$ and $\Delta E_{2p\pi - 2p\sigma} = \alpha(Z_1, Z_2) R^2$ at these b values. Also, the transformation from scattering angle into impact parameter gives an uncertainty at large impact parameters.

Outside of these minor discrepancies, the low-Z data fits the simple scaling law of b very well. The behavior of the high-Z data and especially of the recently observed shift of the adiabatic peak in this scaling law will be discussed in Sec. IV with a new set of data.

III. EXPERIMENTS

The scattered-ion–x-ray coincidence experiments for determination of $P_K(b)$ were performed at the MP accelerator of the Max-Planck-Institut für Kernphysik in Heidelberg. The beams of 54.5- and 90-MeV Ni were collimated to a spot of less than 0.5 mm² and hit Ni, Ge, and Rb solid targets of 5 up to 50 μg/cm² thickness on 10 μg/cm² C backing. The x rays were detected by a Ge(I) detector mounted at 90° relative to the beam axis. The detector solid angle was $\Omega/4\pi = 3.1\%$.

Scattered particles were detected with a 16-ring

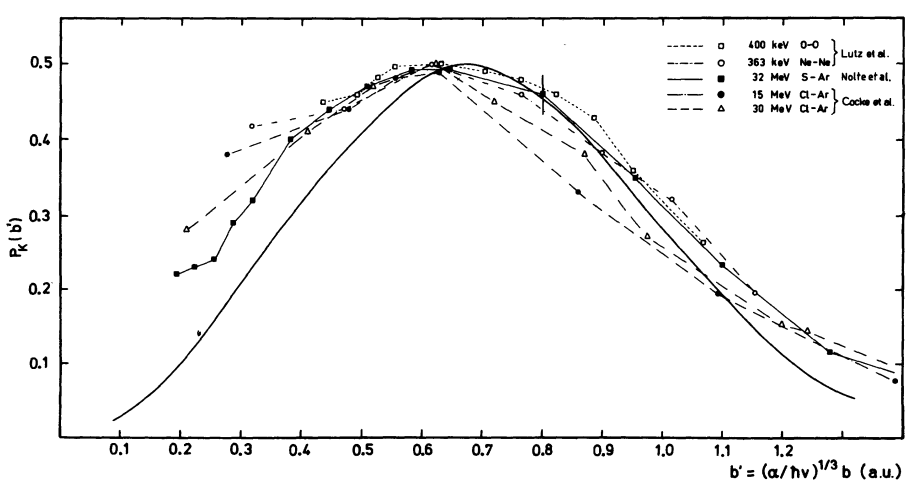

FIG. 1. Normalized K-shell vacancy-production probabilities for $Z_1 \simeq Z_2 \lesssim 20$ as functions of the reduced impact parameter b'. The full line represents the universal solution of $2p\pi - 2p\sigma$ rotational coupling.

parallel-plate avalanche counter.[11] This detector was located at three different positions from the target, allowing us to cover an angular region from $\varphi = 0.2°$ up to 37° with a resolution of $\Delta\varphi/\varphi = 0.1$. A screened potential (Bohr potential) was assumed to convert angles into impact parameters. The coincidence data were taken by event-mode recording, while the total number of detected particles N_p were counted separately. This allowed us to determine the absolute probability for K-vacancy production of one collision partner by

$$P_K^{H,L}(b) = \frac{N_x^{H,L}}{N_T}\,\frac{4\pi}{\Omega}\,\frac{1}{\omega^{H,L}}\,\frac{1}{\epsilon^{H,L}}\,,$$

where N_x is the number of coincidence x rays and $\epsilon^{H,L}$ is the x-ray-detector efficiency. The fluorescence yields $\omega^{H,L}$ were determined according to the procedure given by Greenberg *et al.*,[12] and were taken to be impact-parameter independent. The values we used are $\omega_{\mathrm{Ni}}(54\ \mathrm{MeV}) = 0.53$, $\omega_{\mathrm{Ni}}(90\ \mathrm{MeV}) = 0.58$, $\omega_{\mathrm{Ge}}(54\ \mathrm{MeV}) = 0.63$, $\omega_{\mathrm{Ge}}(90\ \mathrm{MeV}) = 0.68$, $\omega_{\mathrm{Rb}}(54\ \mathrm{MeV}) = 0.72$, and $\omega_{\mathrm{Rb}}(90\ \mathrm{MeV}) = 0.76$. The uncertainty in the fluorescence yield should be smaller than 15%. A possible influence of the target thickness on $P_K(b)$ was investigated by varying the target thickness x from 5 up to 50 $\mu\mathrm{g/cm^2}$. In accord with the results of Annett *et al.*,[7] no influence of target-thickness effects on the shape of $P_K(b)$ was found, only the magnitude of $P_K(b)$ was effected by the target thickness.

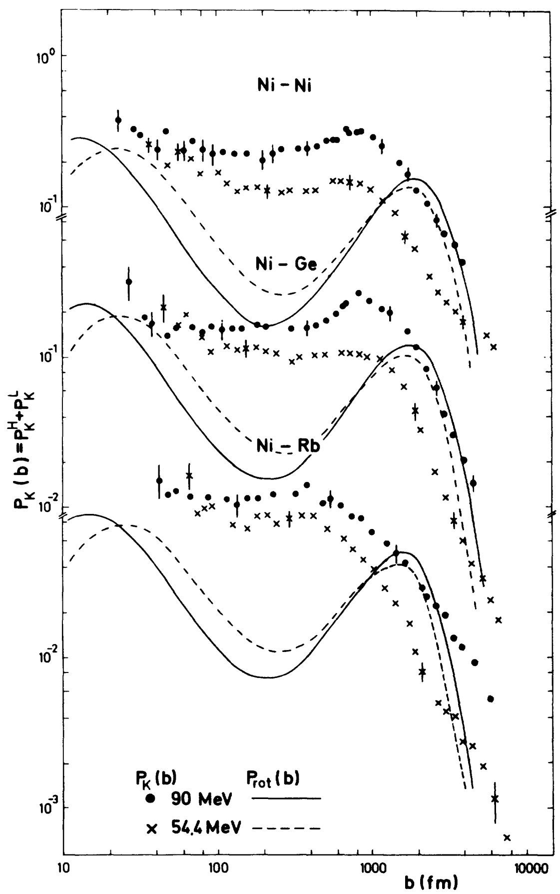

FIG. 2. K-shell vacancy-production probabilities as functions of impact parameter b for the collision systems 54.4- and 90-MeV Ni on Ni, Ge, and Rb. The full and dashed lines represent the prediction of $2p\pi - 2\pi\sigma$ rotational coupling.

IV. RESULTS AND DISCUSSIONS

The measured values of $P_K(b)$ for Ni on Ni, Ge, and Rb are presented in Fig. 2 as functions of the impact parameter b (for $x = 50\ \mu\mathrm{g/cm^2}$). The full line in Fig. 2 represents the prediction of the scaling law of Taulbjerg *et al.*[3] for 90-MeV Ni and the dashed line represents the prediction for 54-MeV Ni as a projectile. The theory is normalized to give the same total cross section σ_K as the data. The total cross sections which we obtained by integrating the measured $P_K(b)$ are listed in Table I. These values agree for Ni + Ni within the error bars of 20% with those taken from Greenberg *et al.*[12] by interpolating to the same energy. All the data show at small b some indication of the rise to the kinematic peak. The position of the calculated adiabatic peak, however, does not agree with the maximum position at about 1000 fm found in the experimental $P_K(b)$ data. This discrepancy is in accord with recent experimental results for 45-MeV Ni + Mn (Ref. 9), 50-MeV Cu + Ni (Ref. 7), 100-MeV I + Ag (Ref. 8), and 143-MeV Nb + Mo (Ref. 10). The existence of a peak at large impact parameters in the $P_K(b)$ data similar to the adiabatic maximum is a strong indication for rotational coupling. The minimum between the kinematic peak and the adiabatic peak is filled in. This filling-in of the minimum was observed also in lighter collision systems $Z_2 \simeq Z_2 \simeq 10$ (Ref. 4) and $Z_1 \simeq Z_1 \simeq 18$ (Ref. 6), and has been interpreted by Meyerhof[13] and by Nolte *et al.*[6] to be due to direct $2p\sigma$ excitation.

To discuss possible reasons for the observed shift between experimental maximum and adiabatic peak, all available high-Z $P_K(b)$ data ($Z_1 \simeq Z_2 \gtrsim 25$)

TABLE I. Total cross sections for Ni on Ni, Ge, and Rb in units of barns (see text).

Ni (MeV)	Ni	Ni (Ref. 12)	Ge	Rb
54.4	31 000	28 000	17 600	7800
90	48 000	52 000	31 000	10 300

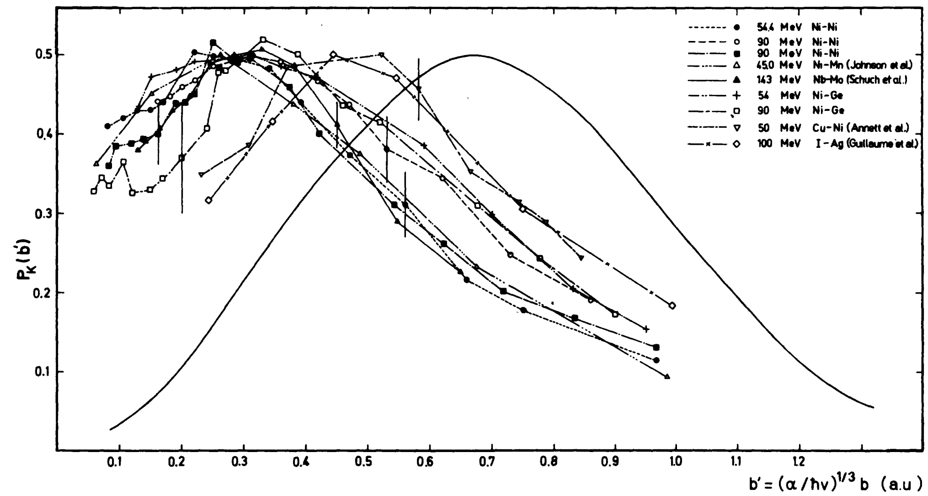

FIG. 3. Reduced $P_K(b')$ for $Z_1 \simeq Z_2 \gtrsim 25$ (see text of Fig. 1).

are plotted as a function of reduced impact parameter b' (Fig. 3). With the exception of Cu + Ni and I + Ag cases, the data again form a common curve. However, the maximum of this common curve is, in comparison with the theoretical universal curve, shifted by about a factor of two to lower b'.

First, we discuss the possible influence of an enhanced $2p\pi$-$2p\sigma$ energy splitting, due to relativistic effects, on the position of the adiabatic maximum. Such an influence has been investigated theoretically by Anholt *et al.*[14] and Jakubassa and Taulbjerg.[15] According to these calculations the relativistic effect has only a small influence on $P_{\text{rot}}(b)$ in the systems considered here. Such an influence should increase with Z. Because the $P_K(b)$ curve of Nb + Mo is falling together with the $P_K(b)$ curve of much lower Z like Ni + Ni and Ni + Mn, and the maximum of the $P_K(b)$ curve of I + Ag is at even larger reduced impact parameters, the presentation of $P_K(b')$ (Fig. 3) demonstrates clearly that the relativistic effect cannot account for the shift of the maximum. Another reason could be the impact-parameter dependence of the $2p\pi$-vacancy production probability $P_{2p\pi}(b)$. This process is assumed to be impact-parameter independent in the region where the $2p\pi$-$2p\sigma$ coupling operates. One distinguishes two processes for $2p\pi$-vacancy production:

(i) Static $2p$ vacancies are brought into the collision either by a double collision process (solid target) or by a highly stripped projectile (gas target).

(ii) $2p\pi$ vacancies are produced on the incoming part of the same collision where rotational coupling occurs.

At the projectile velocities we are considering here, a large fraction of the beam is bearing L-shell vacancies in a solid target (the average charge state of 90 MeV Ni after a solid is about 20^+). Therefore, the $2p\pi$-vacancy production process *i* predominates, and in this case, we can assume that the b dependence of P_K is not influenced by the L-vacancy-producing collisions. Support for this assumption is found in the large (compared with σ_K) L-vacancy-production cross section and in our and Annett's[7] results of the target-thickness dependence of $P_K(b)$, which affects only the absolute height but not the shape of $P_K(b)$.

An experimental indication that even $2p\pi$-vacancy production on the incoming part of the collision (second process) does not affect the shape of $P_K(b)$, was found by Cocke *et al.*[5] for Cl^{n+} + Ar, by Nolte *et al.*[6] for S^{n+} + Ar, and by Hagmann *et al.*[16] for Cu^{n+} on Kr gas targets. Their results show no dependence of the shape of $P_K(b)$ on the projectile-charge state which was varied in order to influence the $2p\pi$-vacancy probability. The influence could be observed in the variation of the absolute height of $P_K(b)$. Also, Hagmann *et al.*[16] found nearly the same shape of $P_K(b)$ as in the very similar collision system Ni + Rb (solid target) presented here. Therefore, it is very unlikely that the observed peak shift is due to solid target effects.

A further reason for the presence of the maximum at smaller b could be rotational coupling to higher-lying orbitals or to continuum states. This channel might become probable in heavier systems, because the $2p\pi$-$2p\sigma$ channel could be closed if the $2p\pi$-vacancy production probability becomes small. However, for the systems investigated here where the projectile carries more than two L vacancies in a solid, this channel should be small compared with $2p\pi$-$2p\sigma$ rotational coupling.

Also, an impact-parameter–dependent anisotropy of K-ray emission by L-shell alignment, which should reduce the K-x-ray emission at 90° at large impact parameters, has been discussed[17] as a possible reason for the peak shift. Because our x-ray detection system has an acceptance angle of about ±20°, this anisotropy must be strongly pronounced to produce the peak shift. One could also hardly obtain the same peak shift for all collision systems and projectile velocities.

In the present stage of theoretical approaches and experimental results concerning the mechanisms of K-vacancy production, one can only speculate about the reason for this shift of the adiabatic peak, and a consistent description of the excitation mechanism, even of the innermost shells, can not be given at present.

V. CONCLUSIONS

With a simple scaling law, derived for the $2p\pi$-$2p\sigma$ rotational-coupling process in the straight-line approximation, we have been able to place all the low-Z ($Z_1 \simeq Z_2 \lesssim 20$) $P_K(b)$ data, in the region of the adiabatic peak, on a common curve. This curve agrees reasonably well with the theoretical universal curve. For the higher-Z case ($Z_1 \simeq Z_2 \gtrsim 25$) the shift of the adiabatic peak, which has been observed recently by different groups and also in the systematic study presented here, shows, within this scaling law, a systematic behavior. Again, all the data form a common curve, but its maximum is shifted by about a factor of two to lower impact parameters compared with the theoretical universal curve.

The existence of an adiabatic peak and its scaling properties suggests that rotational coupling might also be responsible for K-vacancy production in heavier collision systems. The reason for the position of the maximum at a lower b value than predicted by $2p\pi$-$2p\sigma$ rotational coupling could not be clarified. We excluded the relativistic effect as a reason for the peak shift. Investigations of the projectile-charge-state dependence in nearly symmetric collision systems seem to be necessary to clarify the influences of the $2p\pi$-vacancy production process. Also, the measurement of the kinematic maximum may be a helpful tool for getting information about the states which are involved in the K-shell excitation process.

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