Excitation mechanism in the $Na^+ + Ne$ system

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We calculate the polarizations and intensities of the components of the spectral lines Na($3p$) and Ne($2p^5 3p$), and discuss the possible mechanism of their excitation in $Na^+ + Ne$ collisions at high energies. The effect of maximum polarization of the $J = 1 \to J' = 0$ lines is explained.

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A study of the interference structure of the excitation cross section[4] together with the polarization of the radiation[5–7] that is produced when collisions occur in the $Na^+ + Ne$ system makes it possible, in principle, to explain the mechanisms of various excitation processes.

In this paper we attempt to find a correlation between the observed polarization and the intensity of the different components of the spectral lines Na($3p$) and Ne($2p^5 3p$) and the excitation mechanism of these states at high collision energies ($E \gtrsim 10$ keV).

The behavior of the terms that correlate with the considered singly-excited state is determined by the interaction potential of the ionic cores of $Na^+ + Ne^+$, which are split at small distances into Σ and Π terms, so that it is necessary to add the energy of the MO (molecular orbital) of the external electron. It is precisely the splitting $\Delta U \sim 2$–4 eV between the MO levels of the external electron at distances 1.5 a.u. $< R <$ 20 a.u. which is responsible for the interference structure of the cross section.[3–5] We assume that initially, at $R_0 \approx 1.5$ a.u., the system is excited to the lower Σ term (Na^+, Ne^+) of the ionic cores, whereas the external electron can occupy either two σ MO (the σ case) or two π MO (the π case).

In the high-energy limit ($E \sim 10^4$ eV), the calculation of the excitation function is carried out in the following approximation: 1) The trajectories of the nuclear motion are assumed to be straight lines. 2) It is assumed that states with spin $S = 0$ (the spin of the initial state) are produced, and that the spin-orbit interaction of Ne^+(~ 520 cm^{-1}) does not have time to produce a noticeable fraction of triplet states. 3) To calculate the probabilities of the atomic states we use the "sudden approximation," i.e., projection on going from the MO to the atomic states. The corresponding Massey parameter is equal to 0.13 at $E = 10^4$ eV and at an average atomic-level resonance defect on the order of 1500 cm^{-1}. 4) We assume that the orientation of the Σ state of the core (Ne^+) remains immobile in space at distances larger than $R_1 \approx 4$ a.u., starting with which the Σ and Π terms of Na^+Ne^+ are degenerate. This means that at the instant of the transition of the molecular states into atomic states ($R \sim 20$ a.u.) the wave function of the core takes the form $\Psi_{core} = \cos\Theta\Sigma + \sin\Theta(\Pi_{+1} - \Pi_{-1})/\sqrt{2}$, where a tentative value $\sin\Theta = 0.25$ is assumed for $\sin\Theta = R_0/R_1$ in the calculations.

When constructing external-electron MO that are admissible for the initial Σ state of the cores, we took into account the conservation of the total symmetry of the state relative to reflection in the collision plane. For example, for the π mechanism the possible MO is $\pi_x = (\pi_{+1} - \pi_{-1})/\sqrt{2}$.

When light is detected in a direction normal to the beam, just as in[5–7], the intensities of the components with polarization parallel and perpendicular to the beam axis (z), for the $\gamma J \to \gamma' J'$ transition, are equal to

$$I_{\parallel}(\gamma J \to \gamma' J') = k\lambda^3 \langle D_z \rangle^2,$$
$$I_{\perp}(\gamma J \to \gamma' J') = \kappa\lambda^3(\langle D_x \rangle^2 + \langle D_y \rangle^2)/2,$$

where

$$\langle D_i \rangle^2 = \sum_{M'} |\langle \psi^0(\gamma, J) | \hat{D}_i | \psi(\gamma', J', M') \rangle|^2.$$

Here $\psi^0(\gamma, J)$ is the contribution of the state γJ in the initial MO function. $I_{\parallel}$ and $I_{\perp}$ are expressed[8] in terms of the strengths of the corresponding atomic lines,[9] the $3j$-symbols, and the weights $\kappa(\gamma, J)$ of the $L = J$, $S = 0$ structure in the atomic states γJ. The quantities $\kappa(\gamma, J)$, which influence the summary intensity but not the degree of polarization, were calculated with the aid of a Hamiltonian of the type proposed in,[1] which describes well both the levels of the multiplet Ne($2p^5 3p$) and the strengths of the $3p$–$3s$ transition lines.

In the indicated approximation, we calculated the relative intensities $I = I_{\parallel} + I_{\perp}$ and the degrees of polarization $\Pi = (I_{\parallel} - I_{\perp})/(I_{\parallel} + I_{\perp})$ of the components of the $3p$–$3s$ transitions for Na and for the levels p_1, p_2, p_4, p_5, and p_6 of Ne with a noticeable fraction of singlet configuration. The calculation shows that $\Pi(J \to J')$ does not depend on the mechanism for the $\gamma J \to \gamma' J'$ transitions of neon from the states with $J = 1$, and for $J' = 0, 1, 2$ we have respectively $\Pi = -1$, $\Pi = 0.33$, and $\Pi = -0.077$. In full accord with experiment,[5–7] the maximum perpendicular polarization is possessed by the $J = 1 \to J' = 0$ lines. This fact, as well as the independence of Π of the mechanism of the processes, for all the transitions from the state $J = 1$, can be understood even from considerations of symmetry conservation for reflection in the collision plane. Indeed, in such a reflection, the wave function $\psi(\gamma, J, M)$ of Ne goes over into $(-1)^{J-M} \times \psi(\gamma, J, -M)$, so that for $J = 1$ only the state $[\psi(\gamma, 1, 1) + \psi(\gamma, 1, -1)]/\sqrt{2}$ is allowed, whereas the state with $M = 0$, which is responsible for the parallel component of the transition $J = 1 \to J' = 0$, turns out to be forbidden. However, for the lines $J = 3/2 \to J' = 1/2$ of sodium and

Level	p_1	p_2	p_3	p_4	p_5	p_6	p_7	p_8	p_9	p_{10}
$\tilde{I}^{\sigma}$	115	3.3	0	50	4	77	1.4	33	0	0
$\tilde{I}^{\pi}$	9.7	65	0	51	84	77	30	33	0	0
$I^{[7]}_{exp}$	13	46	4	53	41	77	27	44	25	14

$J = 2 \to J' = 1, 2$ of neon, the values of Π are sensitive to the mechanism (σ or π) and are equal respectively to

$$\Pi^{\sigma}(3/2 \to 1/2) = 0.33, \quad \Pi^{\sigma}(2 \to 1) = 0.54, \quad \Pi^{\sigma}(2 \to 2) = -0.92,$$
$$\Pi^{\pi}(3/2 \to 1/2) = -0.43, \quad \Pi^{\pi}(2 \to 1) = 0.29, \quad \Pi^{\pi}(2 \to 2) = -0.35.$$

The degree of polarization Π_{st}, calculated assuming equally probable population of all the atomic states with given J, which are even with respect to reflection in the collision plane, turns out to be $\Pi_{st}(2 \to 1) = 0.12$ and $\Pi_{st}(2 \to 2) = -0.13$ for the transitions from $J = 2$. The two excitation mechanisms differ significantly also in the distribution of the intensities within the multiplet Ne($3p$)Na($3p$). For the σ mechanism, the maximum intensities possessed by the lines $\lambda = 5852$ Å from the level $p_1(J = 0)$, and very low intensity is possessed by the lines from the levels p_2 and p_5 with $J = 1$. At the same time, the population ratio for the π mechanism is reversed for these states. At $\sin\Theta = 0.25$, the distribution of the intensities of the characteristic lines $\lambda_1 = 5852$ Å (p_1), $\lambda_2 = 6163$ Å (p_2), $\lambda_3 = 6717$ Å (p_5), $\lambda_4 = 6096$ Å (p_4), $\lambda_5 = 6143$ Å (p_6), $\lambda_6 = 5890$ Å (Na, $J = 3/2$), and $\lambda_7 = 5896$ Å (Na, $J = 1/2$) takes the form $I_1 : I_2 : I_3 : I_4 : I_5 : I_6 : I_7 = 1.87 : 0.011 : 0.044 : 0.34 : 0.65 : 1.73 : 0.58$ for the σ mechanism and $I_1 : I_2 : I_3 : I_4 : I_5 : I_6 : I_7 = 0.125 : 0.16 : 0.66 : 0.24 : 0.445 : 1.01 : 0.58$ for the π mechanism, respectively.

The table lists a comparison of the calculated (σ and π mechanisms) and experimental[7] relative intensity sums $\tilde{I}(\gamma, J) = \sum_{\gamma' J'} (I_{\parallel} + 2I_{\perp})$ for all the lines that lead to a depletion of the state γJ (the numbers are normalized to the same summary intensity of the radiation from p_6 level as in[7]). Although our approximation does not describe the excitation of the triplet states p_3, p_9, and p_{10}, nevertheless the comparison indicates simultaneous contributions of both the σ and π excitation channels. However, the oscillatory structure can be regarded as due to interference of the π states.

It is of interest to carry out further calculations for lower energies and for all the ion-atom pairs investigated in[7].

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