Monte Carlo calculations of drift velocities of Ne$^+$ ions in helium

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The study of the drift of noble gas ions in gases is a matter of concern due to its importance for applications in gaseous radiation detectors, plasmas, etc. and can be the subject of detailed calculations using Monte Carlo techniques provided the relevant cross-section data, either theoretical or experimental, is available.

In this work, we have applied the Monte Carlo method using a three-dimensional simulation model, based in the work for electrons of Dias et al. (1993), to study the drift of Ne$^+$ ions in gaseous helium, for $p = 760$ Torr and $T = 300$ K, under the influence of an uniform electric field.

The elastic integral and differential collision cross-sections for Ne$^+$ ions with neutral He atoms used in this work were previously calculated (Barata and Conde, 2003), using a modified Tang–Toennies model (Siska, 1986) for the ion–atom potential energy curves of the He–Ne$^+$ interaction with zero crossing distance $\sigma = 1.1591 \times 10^{-10}$ m, well position $r_e = 1.3409 \times 10^{-10}$ m, and well depth $D_e = 0.794$ eV for the X $^2\Sigma_{1/2}$ state (Siska, 1986) and $\sigma = 2.0638 \times 10^{-10}$ m, $r_e = 2.3813 \times 10^{-10}$ m and $D_e = 0.035$ eV for the A$_1$ $^2\Pi_{3/2}$ state (Hausamann and Morgner, 1985). The phase shifts and the scattering amplitude were calculated for these two ground states using the Jeffreys–Wentzel–Kramers–Brillouin (JWKB) semi-classical approximation. If we assume that the Ne$^+$ ions are in the ground state $^2P_{3/2}$, then the states X $^2\Sigma_{1/2}$ and A$_1$ $^2\Pi_{3/2}$ of HeNe$^+$ have equal probability and the corresponding cross-sections have equal weight.

With this model, assuming that all ions are in the ground state, we have calculated the main parameters describing the swarm of Ne$^+$ ions in He gas, namely drift velocities and diffusion coefficients.

We present the results of the calculated drift velocities of Ne$^+$ ions in helium in Fig. 1 for reduced fields E/N from about 3 Td up to about 150 Td using calculated cross-sections. The drift velocities range from 17.3×10^3 to 700×10^3 cm s^{-1}, respectively, and are within about 5% of the experimental values (Ellis et al., 1978), also presented in Fig. 1. Additionally in Figs. 2 and 3 we present results for the standard reduced mobility K_0 (both calculated and experimental) and longitudinal D_L and transverse D_T calculated diffusion coefficients.
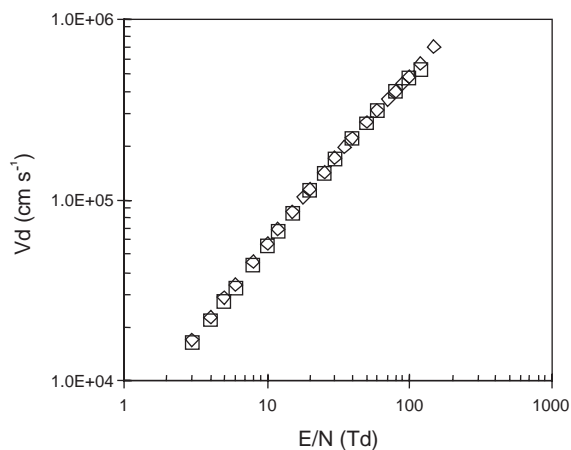

Fig. 1. Calculated drift velocities v_d of Ne$^+$ ions in He gas at 300 K and 760 Torr as function of E/N in Td (Townsends where 1 Td = 10^{-17} V cm^2 per atom): $\diamond$ this work (Monte Carlo); $\square$ experimental data (Ellis et al., 1978).

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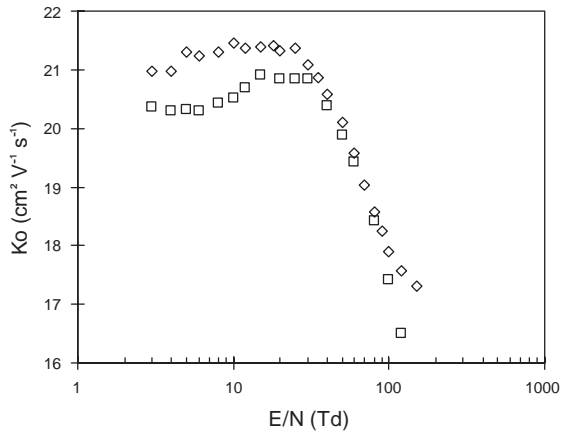
Fig. 2. Standard reduced mobility, K_0 in $cm^2 V^{-1} s^{-1}$, of Ne^+ ions in He gas at 300 K and 760 Torr, as function of the reduced field E/N in Td: $\diamond$ this work (Monte Carlo simulation); $\square$ Ellis et al., 1978 (experimental data).

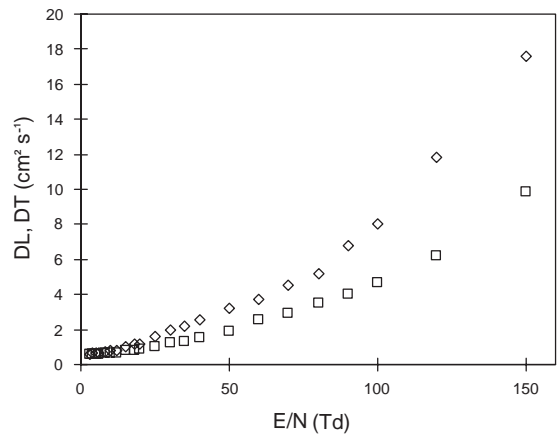Fig. 3. Simulation result (this work) of longitudinal D_L ($\diamond$) and transverse D_T ($\square$) diffusion coefficients in $cm^2 s^{-1}$, for Ne^+ ions in He gas at 300 K and 760 Torr as function of E/N.

References

Barata, J.A.S., Conde, C.A.N., 2003. Calculation of elastic integral and differential collision cross-sections for low energy Ne^+, Ar^+, Kr^+ and Xe^+ ions with neutral He atoms. Radiat. Phys. Chem., this conference proceedings.

Dias, T.H.V.T., Santos, F.P., Stauffer, A.D., Conde, C.A.N., 1993. A Monte Carlo simulation of X-ray absorption and electron drift in gaseous xenon. Phys. Rev. A 48, 2887–2902.

Ellis, H.W., McDaniel, E.W., Albritton, D.L., Viehland, L.A., Lin, S.L., Mason, E.A., 1978. Transport properties of gaseous ions over a wide energy range. Part II. At. Data Nucl. Data Tables 22, 179–217.

Hausamann, D., Morgner, H., 1985. The heteronuclear rare gas ions, a simple model for the determination of the potential curves. Mol. Phys. 54 (5), 1085–1099.

Siska, P.E., 1986. A modified Tang–Toennies model for ion–atom potential curves. J. Chem. Phys. 85, 7497–7498.