Mobility of Kr^+ ions in Kr for cold plasma modelling

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Mobilities of Kr^+ ions in Kr plasma are calculated for both states $^2P_{1/2}$ and $^2P_{3/2}$. Collision cross sections are calculated with quantum and JWKB method by using two different internuclear potential models. The collision cross sections are then used in an optimized Monte Carlo code to obtain mobility over a large range of reduced electric field. Kr^+ mobility values are compared to experimental and previously calculated ones found in the literature. This allows us to identify the most reliable potential model used to obtain cross section. Kr^+ mobility values and diffusion coefficient of this work can be used in kinetic models of low temperature plasma to quantify and improve the active species production for better usage in multiple fields.

1. Introduction

The krypton ion swarm data (reduced mobility and diffusion coefficient) are needed to optimise the plasma jet models in applications such as biomedical or spacecraft propulsion.

2. Potential

In this work, two internuclear Kr^+/Kr potential were used for cross section calculation. The first one (calculated by Kalus et al.[1]) was fitted with a cubic spline curve in order to obtain potential values for all internuclear distances. The other potential was obtained by Bonhommeau et al.[2] by fitting ab initio potential values calculated by Ha et al.[3]. Finally, spin orbit coupling was taken into account by using the Cohen-Schneider semiempirical model[4].

3. Method

Two methods were used to obtain momentum transfer cross section, namely quantum method and semiclassical method (using Jeffreys-Wentzel-Kramer-Brillouin (JWKB) approximation). From these cross sections, Kr^+ mobilities in Kr were obtained using an optimised Monte-Carlo method[5].

4. Results

Figure 1a shows that for $^2P_{1/2}$ state, when the Bonhommeau potential is used, a good agreement is observed between calculated and measured Kr^+ mobility in Kr with a maximum deviation of 3%. However for the $^2P_{3/2}$ state (Figure 1b), the deviation between calculated and measured mobilities is higher than in the case of $^2P_{1/2}$ state, reaching a maximum of 26%. Probably, further improvement of Bonhommeau potential will enhance the agreement with measurements.

The present work improves the agreement between calculated and measured mobilities as compared to previous calculations reported in reference [8].

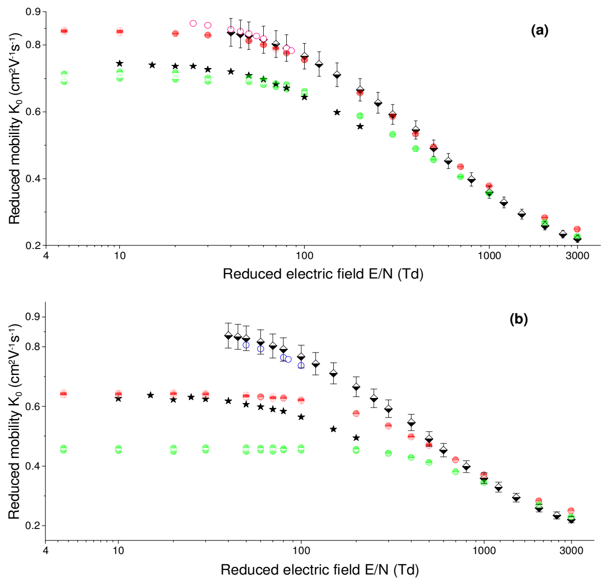

Figure 1: Standard reduced mobility K_0 in $cm^2V^{-1}s^{-1}$ of Kr^+ ions in $^2P_{1/2}$ (a) and $^2P_{3/2}$ (b) state in Kr gas at 293 K and 760 Torr. Exp. value: ○ $^2P_{1/2}$ [6], ○ $^2P_3/2$ [6] and ⬙ not state resolved[7]. Reported calculation: ★ reference [8]. This work: JWKB method: ⊖, ⊖, quantum method: ⊖, ⊖ using potentials of references [1] and [2], respectively.

5. References

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