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SUPRATHERMAL NITROGEN ATOMS AND MOLECULES IN TITAN'S CORONA

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ABSTRACT

Dissociation and dissociative ionization of molecular nitrogen by solar UV radiation and by photoelectrons and sputtering by magnetospheric ions are the main sources of translationally excited (hot) nitrogen atoms and molecules in the upper atmosphere of Titan. The Boltzmann equations describing the production, thermalization, and transport of suprathermal nitrogen atoms and molecules in Titan's upper atmosphere were solved using the Direct Simulation Monte Carlo method. Steady-state energy distribution functions for the hot nitrogen atoms and molecules were calculated vs. altitude in the thermosphere-exosphere transition region. The contribution of dissociation and atmospheric sputtering to the formation of Titan's hot nitrogen corona and to the escape flux into the Saturnian magnetosphere are described using the calculated energy distribution functions. It is shown that photo-dissociation dominates and, therefore, the principal ejecta are N atoms.

INTRODUCTION

The satellite Titan possesses a unique, dense, mainly molecular nitrogen atmosphere and is an important source of neutral atoms and molecules in the Saturnian system (Hunten et al., 1984). For Titan's molecular atmosphere nonthermal mechanisms of particle escape are important (Hunten, 1982; Johnson, 1994). Dissociation of N_2 is a source of suprathermal nitrogen atoms produced by magnetospheric electron impact (Strobel and Shemansky, 1982), by exothermic chemical reactions (Cravens et al., 1997), and by magnetospheric ion sputtering of the upper atmosphere (Lammer and Bauer, 1993). In addition, dissociation and dissociative ionization occur by solar UV radiation and the accompanying photoelectron flux (Shematovich, 1998, 1999). These processes result in the formation of translationally excited (hot, or suprathermal) nitrogen atoms and molecules which populate the corona and contribute to atmospheric escape. Using atmospheric airglow emissions measured by the Voyager UVS experiment, Strobel and Shemansky (1982) estimated an escape flux of 3×10^{26} N atoms per second from Titan. The revised estimate (Strobel et al., 1992) of the nonthermal N atom escape rate of $\leq1\times10^{25}$ sec^{-1} was based on detailed N_2 dissociation rates by magnetospheric electron and photoelectron impact.

In the previous studies (Lammer and Bauer, 1993; Cravens et al., 1997) the production rates of N atoms with energies higher than escape energy (0.34 eV for N atom) were calculated. In estimates of the escaping flux these models were based on an approach which used an exobase - a height strictly dividing collisional and collisionless regions of gas flow. Because the collisional thermalization of the suprathermal nitrogen atoms and molecules is not considered in this approach, the estimates obtained by Lammer and Bauer (1993), and by Cravens et al. (1997) can only be interpreted as upper limits of total nitrogen loss from Titan's upper atmosphere. It has been shown (Shizgal and Arcos, 1996; Marov et al., 1997) that the flux of escaping atoms is typically formed over a wide transition region where the character of the gas flow changes from the thermospheric collision dominated regime to an exospheric collisionless regime. This study is aimed at a detailed investigation of the kinetics and transport of suprathermal nitrogen atoms and molecules in this transition region in Titan's upper atmosphere.

PHYSICAL MODEL

The principal source of suprathermal particles for the exosphere is transport from the atmospheric transition region in which the suprathermal particles are formed and the flow is characterized by velocity distribution functions that vary over both microscopic and macroscopic scales. The following dissociation processes for molecular nitrogen in Titan's upper atmosphere were considered here as important sources of suprathermal N atoms:

(i) The dissociation and dissociative ionization of N_2 by solar UV photons with wavelengths in the range 800-1000Å and by high-energy photo- and magnetospheric electrons. The dissociation processes occur through a predissociation mechanism which implies that a whole spectrum of bound electronic states of N_2 are excited. The excited molecule dissociates into nitrogen atoms in states ^4S, ^2D, and ^2P, and their excess kinetic energy distribution is characterized by a set of discrete peaks at the energies $\Delta E_{ds} = 0.7$ to 1.2 eV and 2 eV (Cosby, 1993). The processes of ionization and Auger ionization of N_2 by soft X-rays with wavelengths in the range 11-50Å were also taken into account (Shematovich, 1998,1999).

(ii) The ion-induced sputtering (Johnson, 1990, 1994; Lammer and Bauer, 1993) of Titan's atmosphere by high-energy ions from the Saturnian magnetosphere occurs via momentum transfer, dissociation, ionization, and charge transfer processes:

$$N_2 + p, N^+, ... \rightarrow \left\{ \begin{array}{l} p, N^+, ... + N_2^* \rightarrow N + N^* + \Delta E_{dis} \\ p, N^+, S^+, ... + N_2^+ + e \\ H, N, ... + N_2^+ \end{array} \right. \qquad (1)$$

Momentum transfer and dissociation collisions with high-energy magnetospheric ions lead to the kinetic energy transfer to the N_2 gas and the formation of suprathermal N atoms. This energy input to Titan's atmosphere causes an additional atmospheric loss. Lammer and Bauer (1993), using a simplified estimate, suggested that this was the dominant loss process. The only observational data on Titan's interaction with surrounding plasma flow are based on the measurements from the single encounter of the Voyager 1 spacecraft with Titan. During the Voyager 1 encounter Titan was inside the Saturnian magnetosphere, and therefore its upper atmosphere was bombarded by magnetospheric protons with energies of about 210 eV and a number density of 0.1 cm^{-3} and by N^+ ions with energies about 2.9 keV and a number density of 0.2 cm^{-3} (Neubauer et al., 1984). This set of plasma parameters was adopted here. In the calculations we use the new collisional momentum transfer and collisional dissociation cross sections for $N+N_2$ and N_2+N_2 collisions from Johnson et al. (2001), and data from Phelps (1991) for other collisional processes. Because the energy transfer in the high-energy $N+N_2$ and N_2+N_2 collisions is strongly dependent on scattering angle distribution we used the calculated differential cross sections for these processes.

NUMERICAL MODEL

An accurate analysis of the processes of production, collisional relaxation, and transfer of suprathermal nitrogen atoms and molecules in the considered transition region of Titan's upper atmosphere can be carried out with the use of the Boltzmann equations (Shematovich, 1999). These equations take into account both the local collisional kinetics and the spatial dynamics of suprathermal nitrogen atoms and molecules and of high-energy nitrogen ions in the transition region and are written as

$$\mathbf{v}\frac{\partial}{\partial \mathbf{r}} f_{Nh} + \mathbf{g}\frac{\partial}{\partial \mathbf{v}} f_{Nh} = Q^{hot}_{Nh} + \sum_{j=N_2,N^+} \sum_{\alpha} J_\alpha(f_{Nh}, f_j) \qquad (2)$$

$$\mathbf{v}\frac{\partial}{\partial \mathbf{r}} f_{N2h} + \mathbf{g}\frac{\partial}{\partial \mathbf{v}} f_{N2h} = \sum_{j=Nh,N_2,N^+} \sum_{\alpha} J_\alpha(f_{N2h}, f_j) \qquad (3)$$

$$\mathbf{v}\frac{\partial}{\partial \mathbf{r}} f_{N^+} + \mathbf{g}\frac{\partial}{\partial \mathbf{v}} f_{N^+} = \sum_{j=N,N_2} \sum_{\alpha} J_\alpha(f_{N^+}, f_j) \qquad (4)$$

Here the $f_j(\mathbf{r}, \mathbf{v})$ is a distribution function for j-species particles by translational and internal degrees of freedom; $\mathbf{g}$ is the gravitational acceleration for Titan; Q^{hot} is a source function for N due to photolytic and electron impact processes; and J_α are the collision terms for elastic, inelastic, dissociation, ionization, and charge transfer collisions (Marov et al., 1997).

This system of kinetic Boltzmann equations is solved using a modification (Shematovich, 1999) of the DSMC method (Bird, 1994). The numerical model includes

(a) The transition region - the height range 600÷1700 km - is divided into a set of radial cells with a characteristic size of the order of the free path length.

(b) In the given set of radial cells the ambient atmospheric N_2 gas is represented by a set of particles with the appropriate altitude profiles for density and temperature.

(c) Using a stochastic modeling method, the evolution of a given set of modeling particles during one time step (~ mean collision time) is determined by the following steps: (i) Suprathermal N atoms are injected at each cell corresponding to the source function Q^{hot} for dissociation. High-energy magnetospheric N^+ ions are injected at the upper boundary with Maxwellian energy distribution with characteristic energy 2.9 keV and physically isotropic entry pitch angle. (ii) For each cell we describe the collisions between ambient atmospheric gas and suprathermal N and N_2, and the high-energy N^+ ions. In the case when Titan is inside the Saturnian magnetosphere the input from proton bombardment is much smaller than from N^+ ions (Lammer and Bauer, 1993); therefore it was not considered in the model. Ejected and thermalized N and N_2 modeling particles are removed from the system. (iii) In the same time step, the dynamics in the transition region for each modeling particle is calculated. (iv) Finally, the statistics of velocity distributions for the suprathermal N and N_2 particles are accumulated.

With this numerical model we obtain the atmospheric density, temperature, and escape flux versus altitude for the suprathermal N_2 and the N.

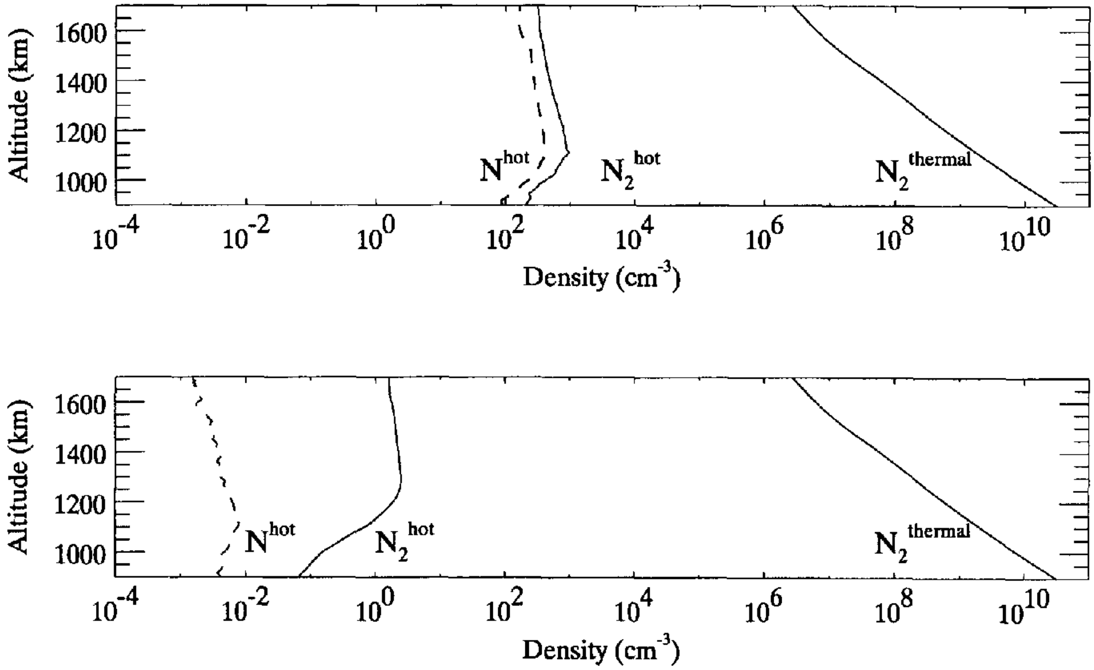

Fig. 1. Density profiles of the hot N_2 (solid curves) and N (dashed curves) formed due to photo-dissociation (top panel) and sputtering (bottom panel).

RESULTS

To study the relative importance of photo-dissociation and sputtering processes for the formation of suprathermal populations of N and N_2 in the upper atmosphere of Titan, we modeled these two sources separately. The production rate and energy spectra of the suprathermal N atoms produced due to the dissociation and dissociative ionization by the solar EUV radiation and by the corresponding flux of photoelectrons were calculated using the model (Shematovich, 1998). In the model the nitrogen atoms and molecules were considered as suprathermal when their kinetic energies are higher than 0.1 eV (e.g., with energies higher then 10-15 thermal gas energies). These fresh, hot nitrogen atoms thermalize in collisions with the ambient atmospheric gas leading to the production of secondary hot nitrogen atoms and molecules. Some of these suprathermal primary and secondary nitrogen atoms and molecules reach exospheric altitudes with kinetic energy greater than the escape energy (0.34 eV for N) and escape to the Saturnian environment. Calculations were made for mean solar activity level $F_{10.7}$=150 and when Titan is inside the Saturnian magnetosphere (conditions for Voyager 1 encounter). In Figure 1 the height profiles of the number densities of suprathermal N and N_2 are shown when the hot particles are produced due to sputtering (bottom panel) and photodissociation processes (top panel). In Figure 2 the mean kinetic energies of suprathermal (kinetic energies higher then 0.1 eV) N and N_2 are given in the top panel. The production rates of the primary and secondary hot N and N_2 formed due to photo-dissociation (middle panel) and sputtering processes (bottom panel) are also shown.

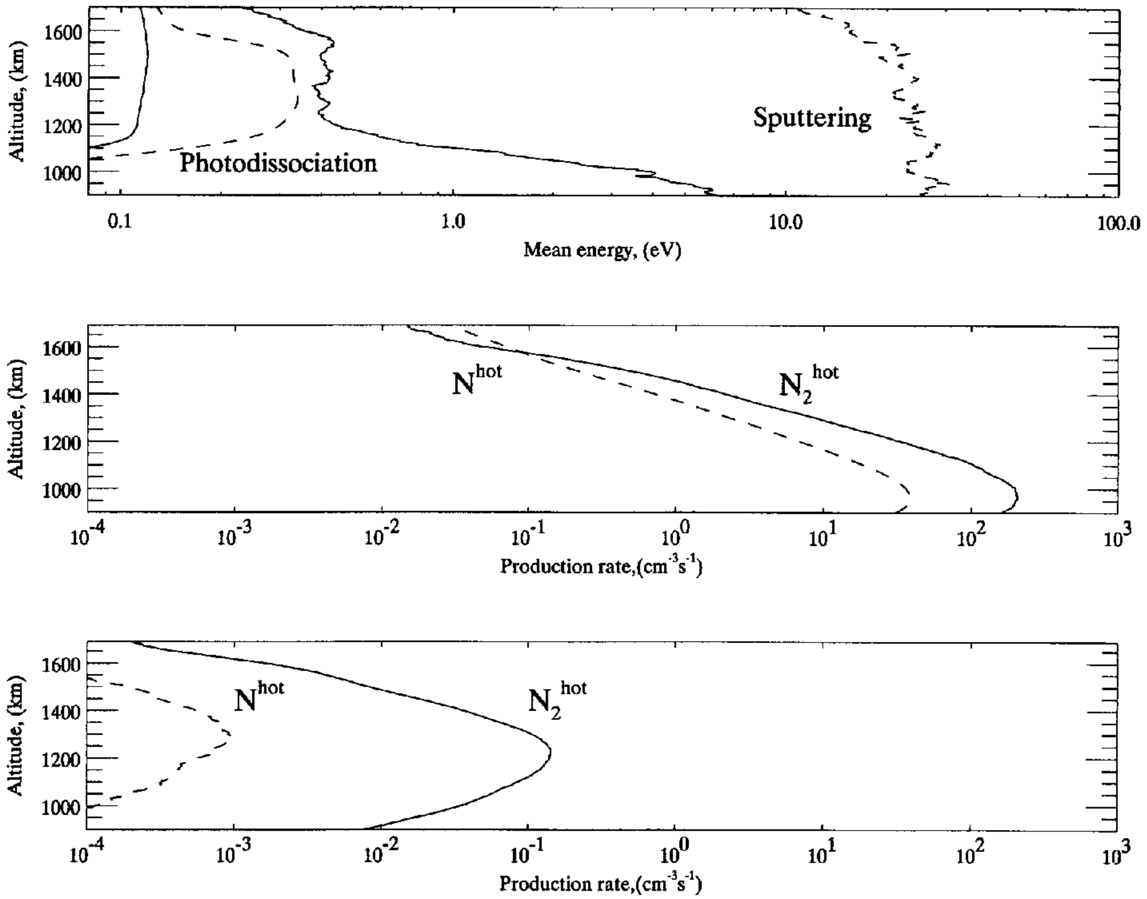

Fig. 2. Top panel: height profiles of mean kinetic energy of hot N_2 (solid curves) and N (dashed curves) due to the photo-dissociation and sputtering processes. Middle panel: production rates of hot N_2 and N due to dissociation processes. Bottom panel: production rates of hot N_2 and N due to N^+ ion-induced atmospheric sputtering.

It seen that elastic thermalization of primary hot N atoms formed due to the photo-dissociation processes cause a significant production of the suprathermal nitrogen in Titan's upper atmosphere. On other hand, bombardment of an atmospheric gas by the high-energy N^+ ions from the Saturnian magnetosphere leads to the formation, through the momentum transfer and dissociation collisions, of both N and N_2 with relatively high kinetic energies (Figure 2, top panel). Although the sputtering production rate of hot N and N_2 is seen to be much smaller than that for the photo-dissociation processes, the hot particles having high kinetic energies produce additional suprathermal nitrogen contributing to the escape flux. The height profiles of total escape fluxes of the hot N and N_2 due to sputtering (bottom panel)and photo-dissociation (top panel) processes are given in Figure 3. Analysis of the calculated escape fluxes of suprathermal N and N_2 shows that the main source of escaping nitrogen in both molecular and atomic form in the sunlit upper atmosphere of Titan is due to the N_2 dissociation by the solar EUV photons and corresponding flux of photoelectrons. Sputtering is a much smaller contribution, and dissociation by magnetospheric electrons is a minor additional source (Keller et al., 1992; Cravens et al., 1997). From Figure 3 it is also seen that the exospheric escape flux is formed in the altitude range 1400 to 1600 km, so that the effective exobase corresponds to these heights.

The total loss of nitrogen is realized in atomic form, in contrast to the results of Lammer and Bauer (1993), and total escape rate can be estimated as $S=\pi\times R_{ex}^2 \times F_{ex}$, where the exobase radius is $R_{ex} \sim (1500\text{km} + R_{Titan})$, and calculated exospheric escape flux is $F_{ex}=6.\times 10^7$ $cm^{-2}s^{-1}$ (see Figure 3). This total escape flux is about $3.\times 10^{25}$ s^{-1} nitrogen atoms per second and strongly depends on the solar activity level and energy input from the magnetosphere.

Our estimate of sputtering loss rate is much lower than value obtained by Lammer and Bauer (1993). The main reason of this difference is that in their study the simplified approach was used: they did not take into account the small angle scattering in the collisions of high-energy nitrogen ions with N_2; thermalization of primary hot nitrogen molecules was not considered. These factors lead to the overestimation of total escape loss rate. The calculated escape rate is close to the revised estimate of Strobel et al. (1992) and to the upper estimate (without taking into account the elastic thermalization of primary hot N atoms) of total nitrogen loss of 2.5×10^{25} s^{-1} due to all photochemical sources (Cravens et al., 1997).

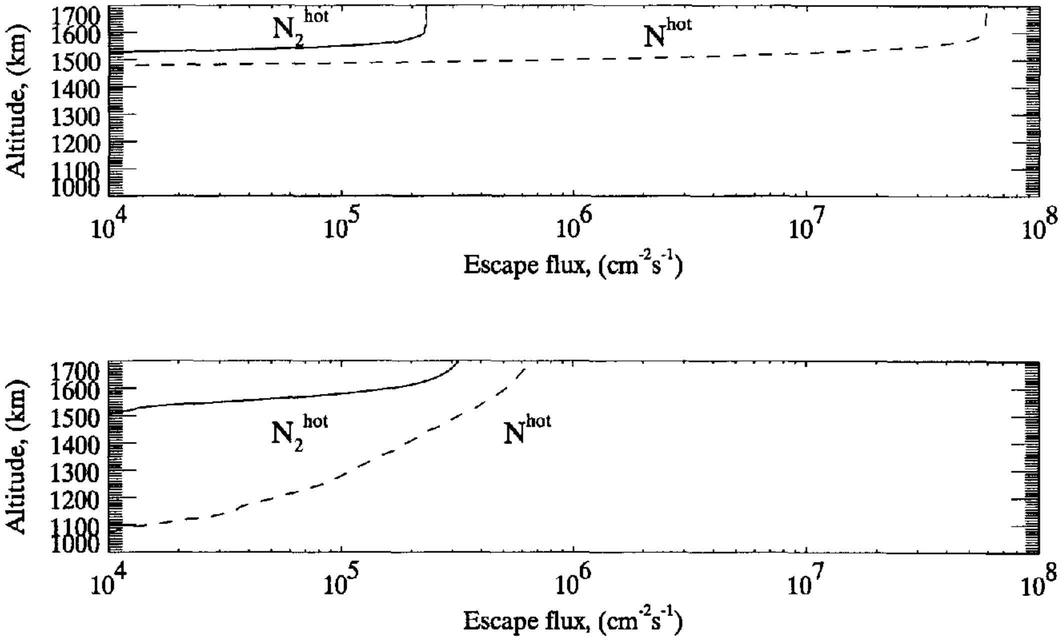

Fig. 3. Escape fluxes of N_2 (solid curves) and N (dashed curves) due to photo-dissociation (top panel) and sputtering (bottom panel) processes.

SUMMARY AND CONCLUSIONS

In this paper we have carried out the first detailed, collisional model of the kinetics and dynamics of suprathermal nitrogen atoms and molecules formed due to photo-dissociation and sputtering processes in Titan's upper atmosphere. It was shown that escape fluxes of N and N_2 are formed in the transition region between thermosphere and exosphere due to the competition between elastic thermalization and hot particle production by photo-dissociation and atmospheric sputtering. We have shown here that N_2 dissociation by solar EUV photons, photoelectrons and incident high-energy plasma all need to be included in describing the hot particle populations in Titan's upper atmosphere and in estimating total nitrogen loss rate - a critical constraint in studies of the evolutionary history of Titan (Lunine et al., 1999). We also showed that the photo-dissociation processes in the sunlit atmosphere are more important than atmosphere sputtering in determining escape and, therefore, atomic nitrogen is the dominant ejecta. This model can be extended to take into account the exothermic ion-molecular reactions in Titan's ionosphere (Cravens et al., 1997). It will be possible to estimate the escaping fluxes of the chemically produced neutrals of the C- and N- families to the Saturnian system.

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