Thermal desorption of molecules from grain surface by accretion shocks: the effect of distribution of desorption energy

*Hitoshi Miura[1], Tetsuo Yamamoto[2], Hideko Nomura[3], Taishi Nakamoto[3], Kyoko K. Tanaka[2], Hidekazu Tanaka[2], Makiko Nagasawa[4]

1.Graduate School of Natural Sciences, Nagoya City University, 2.Institute of Low Temperature Science, Hokkaido University, 3.Graduate School of Science and Engineering, Tokyo Institute of Technology, 4.School of Medicine, Kurume University

Gravitational collapse of a molecular cloud is a transient process to form protostars and protoplanetary disks. The in-falling envelope onto the Keplerian disk often induces accretion shocks at their boundary. Recent ALMA observations suggested sublimation of various molecules, such as SO, from the icy grain surfaces (host grains) at the shocked region [1,2]. The sublimation would considerably affect the chemical environment of the nebula. The shock conditions for the sublimation were calculated numerically in a few papers [3-5]. However, these results were negative for the sublimation of molecules because the shock condition speculated from the ALMA observations is insufficient to sublimate SO molecules from the host grains [4,5].
The numerical models assumed that the desorption energy of a certain molecular species is a single (average) value. However, temperature-programmed desorption (TPD) experiments indicated that the desorption energy is not well represented by a single value because of the heterogeneity of the host grain surfaces [e.g., 6]. If the desorption energy has a deviation from its average value, the sublimation from adsorption sites having smaller desorption energies may occur even by weaker shock heating. In this study, we revisit the desorption fraction when the distribution of the desorption energy is taken into consideration.
Let $f(E_{\rm d})$ be the distribution of the desorption energy, $E_{\rm d}$, of a certain species. The fraction of molecules that have the desorption energies in a range from $E_{\rm d}$ to $E_{\rm d} + dE_{\rm d}$ is given by $f(E_{\rm d})dE_{\rm d}$. The desorption fraction $<P_{\rm d}>$ is calculated by integrating a product of $P_{\rm d}(E_{\rm d})$ and $f(E_{\rm d})$ over $E_{\rm d}$, where $P_{\rm d}(E_{\rm d})$ is the desorption probability of molecules as a function of $E_{\rm d}$. In order to obtain $P_{\rm d}(E_{\rm d})$, we numerically calculate the thermal history of host grains based on the one-dimensional plane-parallel shock-wave heating model [e.g., 7]. In addition, we assume that $f(E_{\rm d})$ is the normal (Gaussian) distribution with the mean $E_{\rm d0}$ and the standard deviation $\Delta E_{\rm d}$. We investigate the dependence of on $\Delta E_{\rm d}$ for various shock conditions.
Let us introduce the numerical results of when molecules adsorbed on 0.1 micron-sized host grains with $E_{\rm d0}$ = 2000 K meat the accretion shock with the pre-shock gas number density of 10^8 cm^{-3} and the shock velocity of 1 km/s. When the desorption energy has no deviation ($\Delta E_{\rm d}$ = 0 K), we obtain $<P_{\rm d}> = 1.7\times10^{-9}$. $<P_{\rm d}>$ increases with the increase of $\Delta E_{\rm d}$: = 1.7×10^{-8}, 1.7×10^{-5}, and 1.5×10^{-2} for $\Delta E_{\rm d}$ = 100, 200, and 400 K, respectively. The deviation of the desorption energy increases the desorption fraction of molecules by orders of magnitudes. This result suggests that molecules adsorbed on the host grains in molecular clouds can desorb more easily than that expected before.
References: [1] N. Sakai et al. (2014), Nature 507, 78. [2] H.-W. Yen et al. (2014), ApJ 793, 1. [3] D. A. Neufeld and D. J. Hollenbach (1994), ApJ 428, 170. [4] T. Aota et al. (2015), ApJ 799, 141. [5] H. Miura et al. (2015), Japan Geoscience Union Meeting 2015, abstract PPS24-11. [6] T. Hama and N. Watanabe, 2013, Chem. Rev. 113, 8783. [7] H. Miura et al. (2010), ApJ 719, 642.

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