

# Status report of diamondoids as alternative propellants for ion-thrusters

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**Abstract:** Diamondoids are a class of molecules which are of a diamondlike structure. Derivates of this class are possible candidates for replacing resource-critical xenon as propellant for ion-thrusters. Results on the progress of tests using adamantane, which is the smallest diamondoid  $C_{10}H_{16}$ , will be discussed. The focus of the investigations is on the fragmentation of the molecule and first performance mappings using a RIT-type thruster. The dependence of the fragmentation on the operating point also has been studied. A strategy for experimentally identifying molecules which are alternatives for replacing xenon as propellant will be given.

## Nomenclature

$\dot{m}_0$	= exhausted mass flow of the molecule
$v_{\text{ex}}$	= velocity of extracted particles
$F_0$	= thrust without fragmentation of the molecule
$e$	= elementary charge $1,602 \cdot 10^{-19}$ C
$U$	= effective extraction voltage
$I_{\text{sheath}}$	= current reaching the plasma sheath
$T_e$	= electron temperature
$x$	= degree of fragmentation
$y$	= ratio of the mass of a fragment to the mass of the original molecule
$I_{\text{beam}}$	= beam current
$P$	= power
$I_{\text{SP}}$	= specific impulse
$\Delta v$	= characteristic velocity increment of a mission
$\Delta E$	= energy resolution
$\Delta m$	= mass resolution

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## I. Introduction

WHEN using molecular propellants, one of the most critical aspects in terms of suitability, is the fragmentation of either the molecule or the molecule-ion, as fragmentation will lead to a change of thrust-efficiency and will reduce the lifetime of the thruster.

Diamondoids are  $sp^3$ -hybridized hydrocarbons. Up to now, only the smallest diamondoid, so called adamantane  $C_{10}H_{16}$ , was tested as propellant. The arrangement of carbon-atoms resembles a fraction of the diamond crystal lattice and the molecule as a whole is almost spherical. Hydrogen terminates the dangling bonds of the diamond lattice fragment. A general overview of preferable properties of propellants was given in Ref. 6. While adamantane is of a similar mass than xenon, higher diamondoids may be much heavier. While the light diamondoids (adamantane, diamantane, triamantane) can be synthesized efficiently, heavy diamondoids (tetramantane, pentamantane etc.) are a by-product of the oil-industry<sup>7</sup>. Another potential alternative for replacing xenon as propellant is iodine<sup>8</sup>. In contrast to the halogen iodine, diamondoids are not very reactive. The focus here is on the use of diamondoids with gridded-ion-thrusters (GIT), especially radio-frequency ion-thrusters (RIT). However, many of the basic thoughts can also be applied to Hall-effect-thrusters (HET). In section II the effect of fragmentation on performance will be discussed. Section III briefly shows the setup used to investigate the ion-beam, while the results of the measurements are given in section IV.

## II. Impact of fragmentation on thrust and power efficiency

Let us consider a propellant molecule of mass  $m_0$  and a total mass flow  $\dot{m}_0$  of these molecules. We will analyse two limiting cases, in a simplified picture in order to understand possible impact of fragmentation on thruster performance.

First, no fragmentation of the molecule takes place. All the propellant molecules are singly charged and accelerated with a voltage  $U$  in the extraction process yielding an exhaust velocity  $v_0 = \sqrt{2eU/m_0}$  and, thus, a total thrust  $F_0 = \dot{m}_0 v_0$ . The power needed to generate the total thrust is given by  $P = UI_{\text{beam}} = P_0$  where  $I_{\text{beam}} = (e/m_0)\dot{m}_0 v_0 = I_0$ .

Second, all molecules are fragmented in the same way. Each molecule is split into two fragments one of mass  $m_1 = y m_0$  and the other of mass  $m_2 = (1 - y)m_0$  whilst the mass flow is the same as before with  $\dot{m}_0 = y \dot{m}_0 + (1 - y)\dot{m}_0$ . The parameter  $y$  takes meaningful values in the range  $0 \leq y \leq 0.5$ . Again, both fragments are singly charged and all fragments are extracted with voltage  $U$  yielding exhaust velocities  $v_1 = v_0/\sqrt{y}$  and  $v_2 = v_0/\sqrt{1 - y}$ . As the total thrust is given by the sum of the thrusts generated by the two types of fragment molecules, one finally obtains

$$F(y) = \left( \sqrt{y} + \sqrt{1 - y} \right) F_0. \quad (1)$$

Taking into account that both singly charged fragments contribute to the beam current instead of just the singly charged molecule, one obtains  $I_{\text{beam}} = I_1 + I_2 = 2I_0$ . Thus, the power needed to generate this thrust is  $P = 2P_0$  and independent of  $y$ .

Based on these two limiting cases, we may discuss the case where only a fraction  $x$  of the molecules is split into fragments. The corresponding expressions for the total thrust and the required power as a function of  $x$  and  $y$  are given by:

$$\begin{aligned} F(x, y) &= (1 - x)F_0 + x(\sqrt{y} + \sqrt{1 - y})F_0 \\ P(x) &= (1 - x)P_0 + 2xP_0 \\ \frac{P(x)}{F(x, y)} &= \frac{P_0}{F_0} \frac{1 + x}{1 - x + x(\sqrt{y} + \sqrt{1 - y})} \end{aligned} \quad (2)$$

Curves of the thrust and power-to-thrust ratio versus the degree of fragmentation  $x$  are plotted in Fig. 1 for different  $y$ . Both quantities are given in units  $F_0$  and  $P_0/F_0$  corresponding to the first case where no fragmentation of the molecule takes place in the extraction process. It can be seen that for the assumptions made, fragmentation always yields an increase of thrust. However, this increase of thrust is always accompanied by a decrease in thrust efficiency, i.e. an increase in power-to-thrust ratio. Furthermore, it turns out that fragmentation into two fragments of equal mass  $m_0/2$  for  $y = 0.5$  is most favorable. In case of full fragmentation  $x = 1$  one can achieve a thrust of  $\sqrt{2}F_0$  for the price of an increase of power-to-thrust ratio to  $\sqrt{2}(P_0/F_0)$ .

In general, dissociation into fragments, though increasing the thrust achievable, leads to a loss of thrust efficiency. The thrust in a mission scenario is either limited by the electric power or by the total propellant mass available. In case of attitude or altitude control of a satellite, the consumable electric power is likely to be the limiting factor and a low degree of dissociation of propellant molecules is desirable. On the other hand, for deep space missions the spacecraft will probably be powered by a small nuclear reactor instead of solar arrays. In such a case, electric power may be much less restricted and available propellant mass is the dominant limitation. In this scenario a high specific impulse  $I_{SP}$  to reach a high  $\Delta v$  can be more important than thrust efficiency. Therefore, a dissociation of the propellant may be advantageous in missions demanding an extraordinary high  $\Delta v$ .

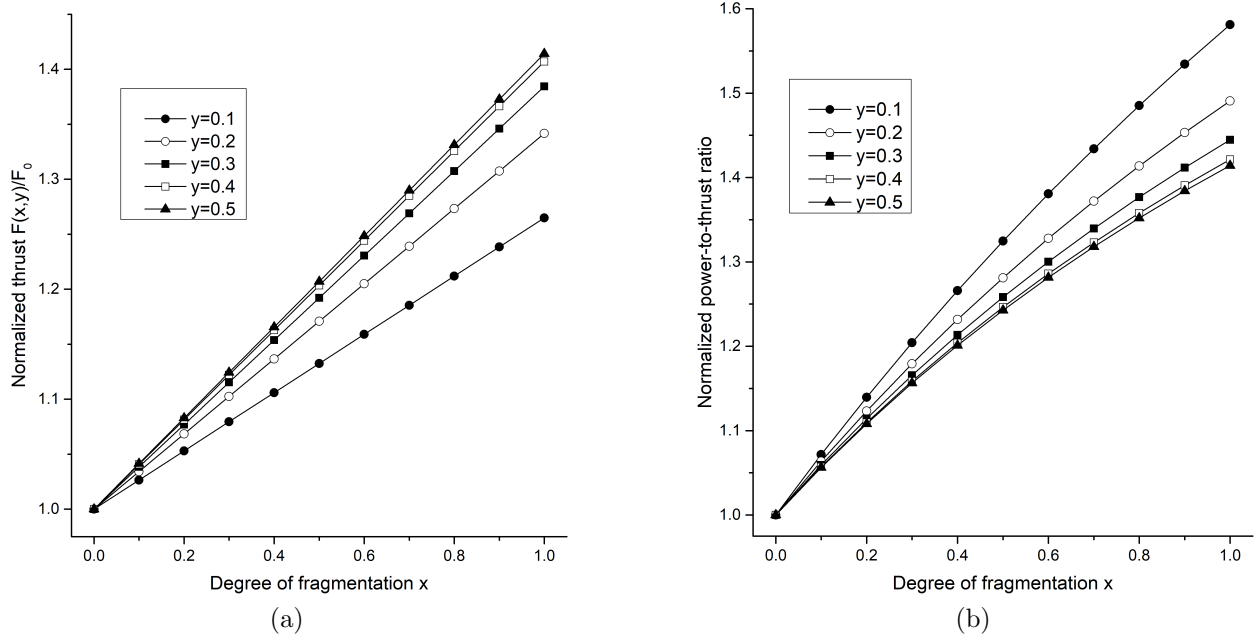


Figure 1. (a) Total thrust and (b) power-to-thrust ratio as a function of degree of fragmentation  $x$  of a molecule into two singly charged fragments of masses  $y m_0$  and  $(1 - y)m_0$ , respectively, for different  $y$  values.

### III. Experimental setup

#### A. Mass spectrometer

The fragmentation of adamantane was investigated with a sector mass spectrometer. A scheme of the setup is shown in Fig. 2. A RIT-10-type thruster, but with a reduced number of beamlets, was chosen as ion source. The mass conductivity of the grid was reduced to match the maximum adamantane flow of 2 sccm. The slits before and after the bending magnet can be used to reduce the transverse components of the ion-beam to gain a better resolution of the mass spectra. In case of adamantane, the slits were almost entirely open to provide sufficiently strong signals. This is very useful to study the spectra of ions extracted of the thruster even if the grid voltages are set to 0 V. The magnet can provide a maximum flux density  $B$  of  $\approx 1$  T which is sufficient for measuring ions up to  $2.5 \text{ MeV} \cdot \text{u}$ . A Faraday-cup is used as current-detector, a Keithley Picoampèremeter 6485 is performing the readout. A secondary-electron-repeller is installed.

**RESOLUTION OF THE SPECTROMETER** One has to take into account that a very high resolution of the spectrum is not achievable since oscillations of the sheath of the rf-driven plasma lead to energy-fluctuations  $\Delta E$  in the order of some 10 eV. This effect limits the effective mass resolution. For a spectrometer using a dipole magnet one can show, assuming a symmetric  $\Delta E$ :

$$(\Delta m/m)/(\Delta E/E) = (2 \cdot E^2)/(E^2 - (\Delta E)^2) \geq 2. \quad (3)$$

For example, for an adamantane-ion (136 u) at a extraction voltage of  $U = 1 \text{ kV}$  and  $\Delta E = 20 \text{ eV}$  the best achievable resolution is  $\Delta m = 5.44 \text{ u}$ . Therefore, a loss of a hydrogen-atom or ion cannot be resolved while

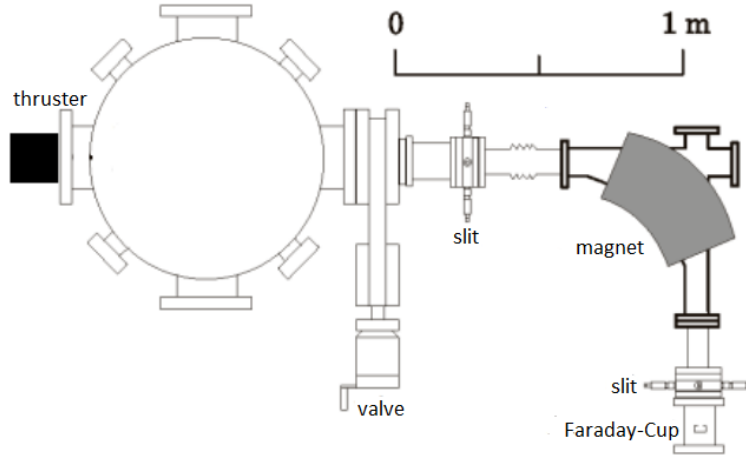


Figure 2. Setup for measurements of the ion-beam mass spectrum

a loss of carbon can be detected in principle. An expected fragmentation channel of adamantane-ions is the loss of a hydrogen atom, since the fragmentation energy is only about 1.4 eV larger than the ionization potential.

## B. Test-facility

The cylindrical vacuum-chamber has a volume of roughly  $0.5 \text{ m}^3$ . The total pumping speed for adamantane and xenon was calculated to be about 14000 l/s. The calculated value was confirmed with a xenon coldflow test. The indicated pressure with adamantane is typically in the low to mid  $10^{-3} \text{ Pa}$  range. The real pressure is assumed to be significantly lower. The thruster is directly attached to a flange of the chamber and can be controlled by a measurement software written in Labview. One advantage of attaching the thruster to a flange, instead of placing the ion source in the vacuum-chamber, is a much easier heating of the gas supply lines.

The flow is controlled with a MKS-1150-MFC (mass-flow-controller). The controller can be heated up to  $150^\circ\text{C}$  to avoid resublimation. The vapor pressure is monitored by a heatable, capacitive gauge, which is independent of the the gas type used. Typical pressures are  $\approx 2 \text{ kPa}$ . The much lower inlet pressures in comparison to usual xenon-flow control-units requires much larger piping dimensions. Even for a rather small flow of 2 sccm an outer diameter of at least 6 mm or a quarter inch should be used. A 5 cm long  $1/8''$  pipe already reduced the flow by several percent. Therefore, it was necessary to design a new plasma-resistance to avoid a discharge in the feeding-line without disturbing the flow-regulation. The resistance consists of a rather large quartz-glass-pipe ( $9/16'' \approx 14,3 \text{ mm}$  diameter) filled with quartz-wool.

## IV. Experimental results

### A. Fragmentation

We started the study of the fragmentation by measuring the adamantane-spectra at different flows. The RFG (radio-frequency-generator) input power remained constant. An example is given in Fig. 3 (a).

Since the broadness of the peaks varies with the mass one has to determine the area of each peak for a better comparison of intensities (see Fig. 3 (b)). A relatively low screen-voltage was chosen to avoid arcing inside the extraction system.

Despite the correction of the spectra the relative abundance of light hydro-carbons is much higher than anticipated. A previous investigation of the fragmentation with a ECRIS (electron-cyclotron-resonance-ion-source) showed less fragmentation at a neutral pressure of  $3 \cdot 10^{-2} \text{ Pa}$  <sup>6</sup>. The neutral gas pressure in the RIT was assessed to be in the order of a few  $10^{-1} \text{ Pa}$ . Furthermore, the fragmentation barely changes with

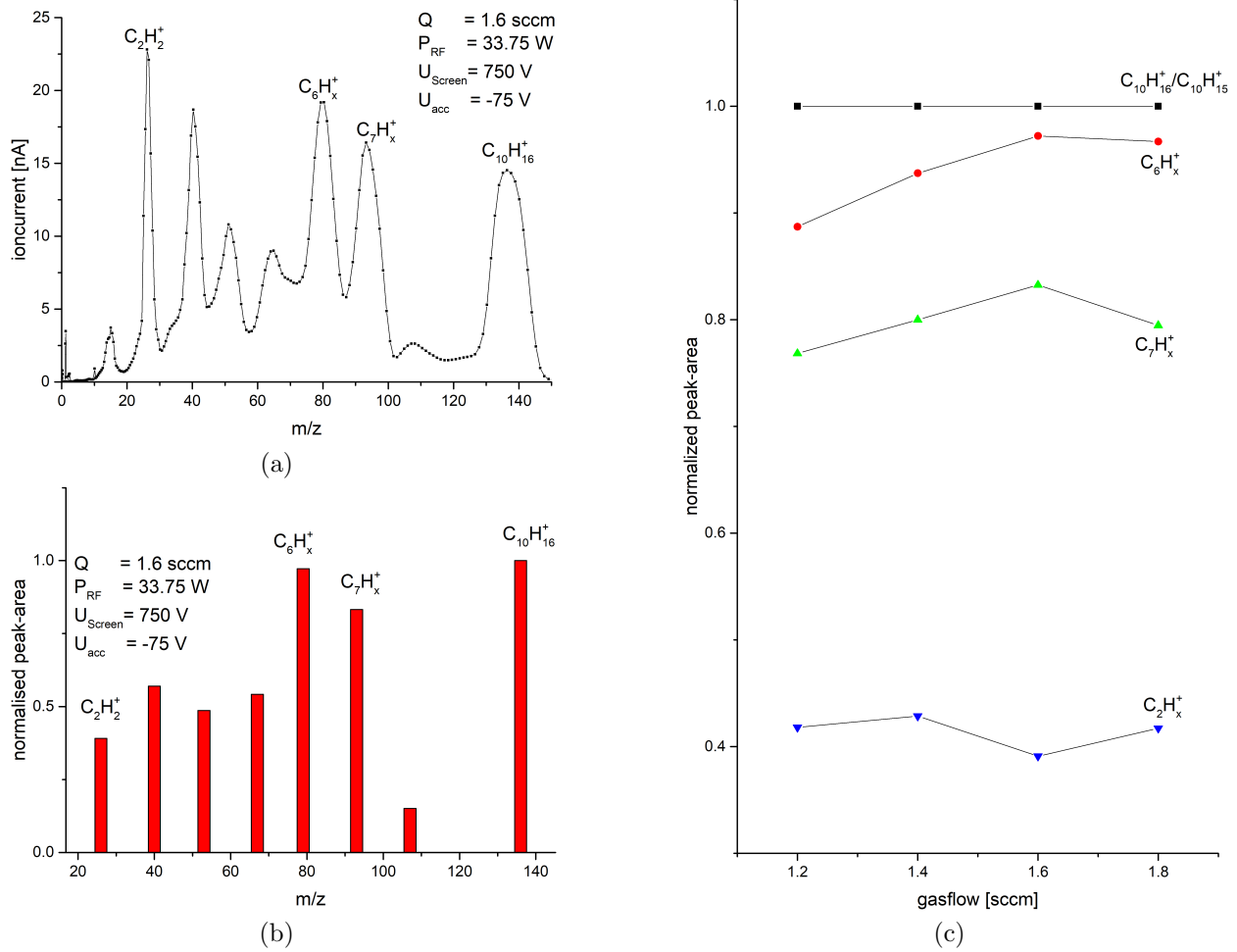


Figure 3. (a) Example mass spectrum of the extracted ion-beam of a RIT-10-type thruster using pure adamantane, (b) Relative intensity of adamantane and fragments of the extracted ion-beam of a RIT-10-type thruster using pure adamantane and (c) Fragmentation of adamantane as function of the gas flow. The dc-input-power of the RFG remained constant.

variation of the gas flow (Fig. 3 (c)). This means that slight changes of the electron temperature do not influence the fragmentation much.

One possible explanation for this behavior is a multiple-step fragmentation of adamantane. If this is the case, a change of rf-power and, therefore, electron density should show a stronger influence on fragmentation. Electron-impact ionization cross sections of hydro-carbons are typically rather large. Even for the relatively small acetylene ( $C_2H_2$ )-molecule the maximum cross-section<sup>3-4</sup> of  $(400 - 500) \cdot 10^{-16} \text{ cm}^2$  is similar to that of xenon<sup>5</sup>. Thus, this explanation may be plausible. First measurements of the rf-power-dependence have been performed without extraction voltages to avoid arcing-issues. If no voltage is applied to the thruster grids, the ions will be accelerated by the sheath potential solely. This leads to a bad resolution of the spectra. Therefore its hard to distinguish various hydro-carbons. Nevertheless, an increase of the relative abundance of light hydro-carbons with increasing rf-power can be observed.

Mass spectra can be used to estimate the electron temperature of the plasma. The position of the peaks is dependent on the sheath-potential and, therefore, the electron temperature. First results show a higher electron temperature of a adamantane plasma in comparison to a xenon-plasma. Even with a adamantane-flow more than 5 times higher compared to the xenon-flow, the estimated temperature was approximately 1 eV higher and amounts to approximately 7 eV at a flow of 1 sccm. Assuming a Maxwellian electron energy distribution function and an electron temperature of 7 eV, the probability for a 20 eV-electron compared to that for a 10 eV-electron is only about 50 % smaller (figure 4). The relative abundance of the electrons with an energy smaller than the ionization energy is 38.2 %, electrons with an energy between ionization threshold and fragmentation threshold have a relative abundance of 6.6 % only and electrons with sufficient energy for fragmentation a relative abundance of 55.2 %. This means that either the gap between ionization-threshold and fragmentation threshold must be increased considerable or the cross-section for fragmentation must be significantly reduced in order to avoid strong fragmentation. Both requires a modification of the molecule, i.e. chemical engineering.

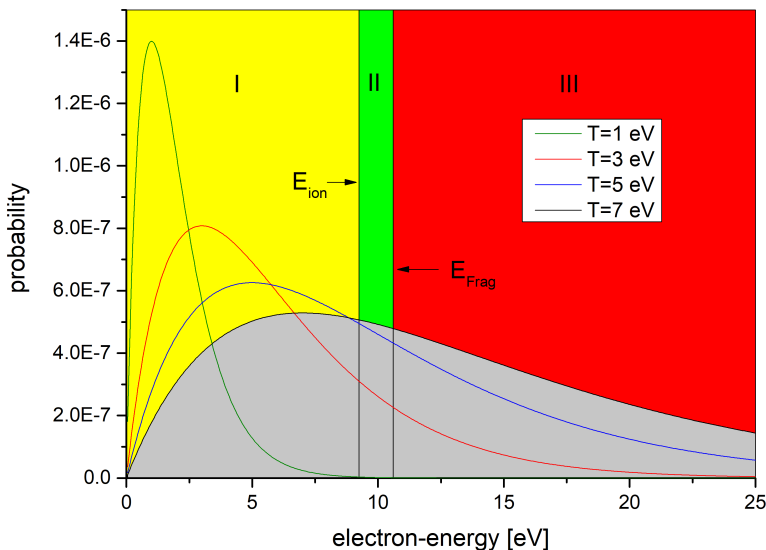


Figure 4. Maxwell-Boltzmann-distributions for four electron-temperatures. The yellow area (I) indicates energies too low for ionization and fragmentation, the green area (II) energies sufficient for ionization only and the red area (III) energies sufficient for both ionization and fragmentation.

## B. Performance

In addition to fragmentation studies, the thrusters performance with adamantane as propellant was investigated. The chosen method was a performance mapping, which is a standard method for several decades to characterize RITs. While the grid-voltages are kept constant, the gas flow as well as RFG-input-power are varied in such a way, that the extracted current remains constant. For xenon, it can be assumed that the produced thrust  $F$  remains almost constant as well. This may be not true for adamantane due to changes of fragmentation, especially with varying RFG-power, leading to a change in average mass of the extracted ions. As Fig. 5 (a) shows, the shape of the performance curves for adamantane is similar to those of xenon. How-

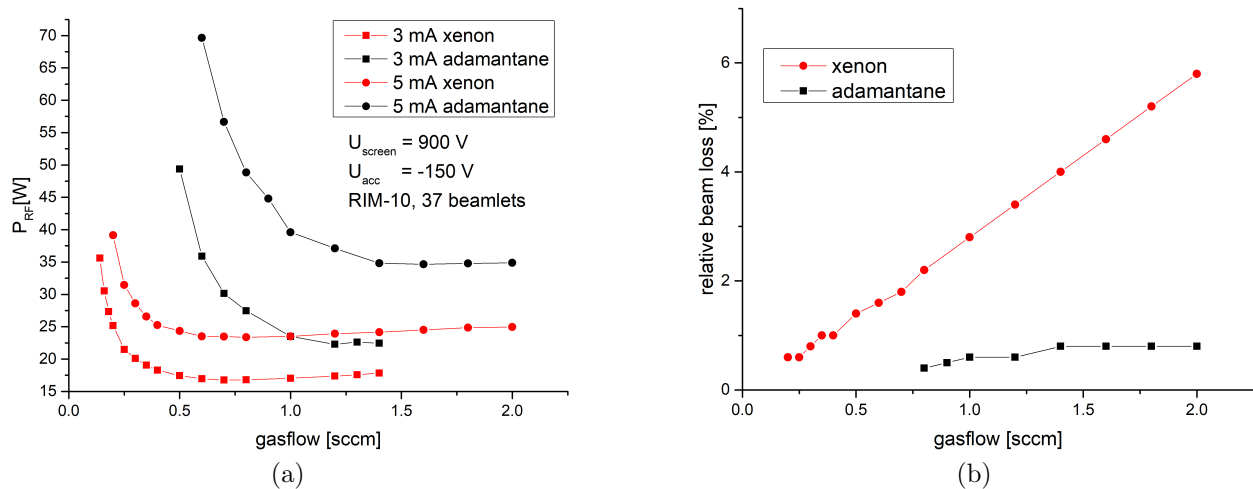


Figure 5. (a) Performance mapping for xenon and adamantane for two extraction currents and (b) relative beam loss with xenon and adamantane as function of the gas flow at a beam current of 5 mA

ever, the necessary flow as well as the required RFG input power are significantly higher compared to xenon. A positive aspect is the much smaller loss of beam current at the acceleration grid at comparable flows, see Fig. 5 (b). Due to the almost constant slope of the beam loss with xenon it is assumed that the losses are mainly driven by charge-exchange-processes. This will potentially lead to a increase of thruster-lifetime, if arcing can be avoided.

## V. Issues with adamantane

One major issue driving the RIT-type thruster with adamantane is the appearance of amorphous carbon layers in the grid system. This leads to arcs and therefore an unstable extraction of the beam. Additionally the plasma has the tendency to break down without any visible previous instability. A possible explanation for this phenomenon is the appearance of negatively charged nano-particles. One common procedure to produce carbon-nano-particles is the usage of an acetylene-plasma. As shown in Fig. 3 (a), the acetylene-ion appears in the beam. Furthermore, neutral acetylene was detected with a residual gas analyzer, when the thruster was operated with adamantane. Negative ions were detectable in the mass spectra of the beam as well. A similar problem with a quenching plasma occurred in the past with fullerenes as molecular propellant<sup>2</sup>.

## VI. Conclusion and Outlook

The fragmentation of adamantane was investigated. A much stronger fragmentation as originally expected was observed. While the exact reasons for the unexpected harsh plasma conditions are not fully understood yet, it has become clear that the energy-gap between ionization energy and fragmentation-energies is too narrow, especially if a Maxwellian distribution of electron energies is given. Thus significant fragmentation cannot be avoided. If fragmentation may be avoided, the amount of energy loss channels can be lowered, allowing a much better performance.

In future investigations, we will chemically engineer diamondoids in order to increase the gap between ionization and fragmentation energy. Before testing the propellant in a thruster, the propellant will be analyzed with a DETOF (Delayed extraction time of flight)-experiment. The purpose of this experiment is to measure total electron-impact-ionization cross sections as well as fragmentation cross sections. One advantage of this experiment is that the fragmentation of a molecular propellant can be directly correlated with the electron energy. Furthermore, only tiny amounts of the substances are required and an assessment of the fragmentation of the molecule on electron impact can be quickly performed. Thus, this approach allows us to screen a large number of candidate molecules in a short period of time.

If a suitable propellant candidate is found, the candidate molecule will be tested as propellant inside the

thruster as described in this paper.

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