A-857

Molecular Dynamics Simulations of Nanodroplet Break-up for Ionic Liquid Electrospray Thrusters

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1. Introduction

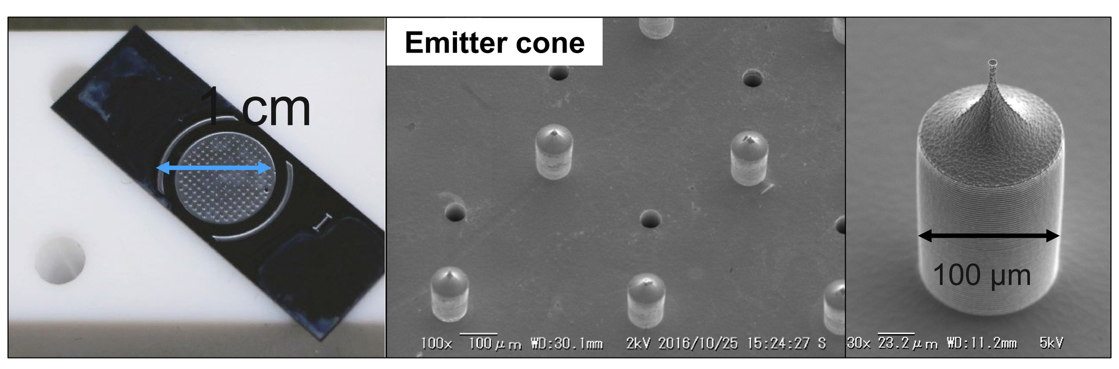
Microsatellite (< 50 kg)

- The launched number of microsatellites has increased recently.
- The development cost is lower and the development period is shorter than the conventional satellites.

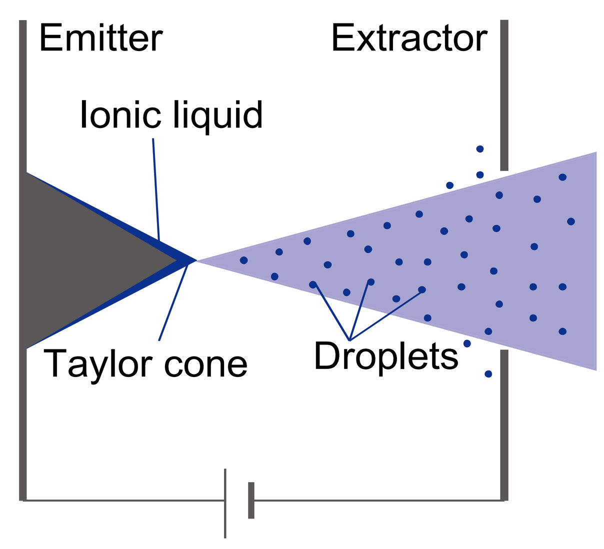
➡ It is useful for universities and small companies. However, it is difficult to mount conventional thrusters.

Ionic liquid electrospray thrusters (ILESTs)

- It is very simple structure and mainly consists of an emitter and an extractor.
- The emitter size is on the order of micrometers or less.



Nakagawa, K., et al., *Jpn. J. Appl. Phys.* 56 (2017) 06GN18.

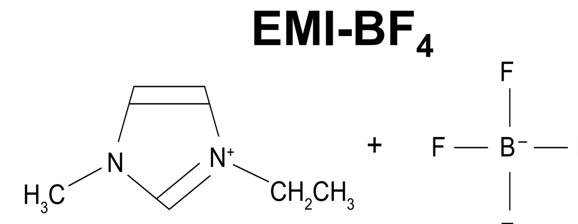


Propellant : Ionic liquid

- The liquid contains only ions without solvent.
- The liquid can exist as liquid even in vacuum.

➡ High-pressure gas systems are unnecessary for ILESTs. Ionic liquid is one of the most suitable propellant for microsatellites.

EMI-BF$_4$



Objective

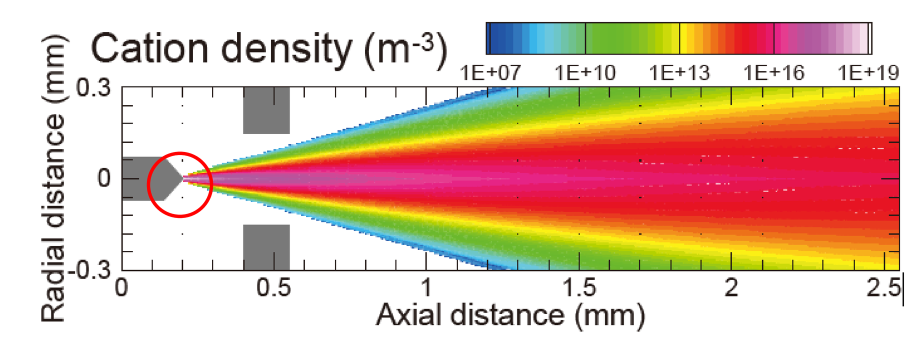
- Some of the divergent ion beams collide with the extractor, which could lead to an erosion of the extractor. As a result, it leads to short life.
- It is difficult to measure in experiments because of the small size.

Previous study

Ion trajectories were determined by boundary conditions at the emitter tip, which were **the kinetic energy** and **the extracted angles**.

The kinetic energy and the extracted angles at the emitter tip had to be assumed **in the particle simulation**.

We have conducted **molecular dynamics simulations** in order to get the kinetic energies and the extracted angles accurately.



Emoto, K., Tsuchiya, T., and Takao, Y., *Trans. JSASS, Aerosp. Tech. Japan.* 16 (2018), pp.110–115.

2. Numerical Method

Molecular Dynamics (MD) simulation

- Molecular dynamics can simulate **atomic-scale phenomena**, which considers intra- and inter-molecular forces.
- We can self-consistently obtain **the kinetic energy** and **the extracted angles** from the characteristics of ions and applied electric field.
- The force is from potentials such as Lennard-Jones potential and Coulomb potential.

$$\boldsymbol{F} = -\frac{d\phi(\boldsymbol{r})}{d\boldsymbol{r}}$$

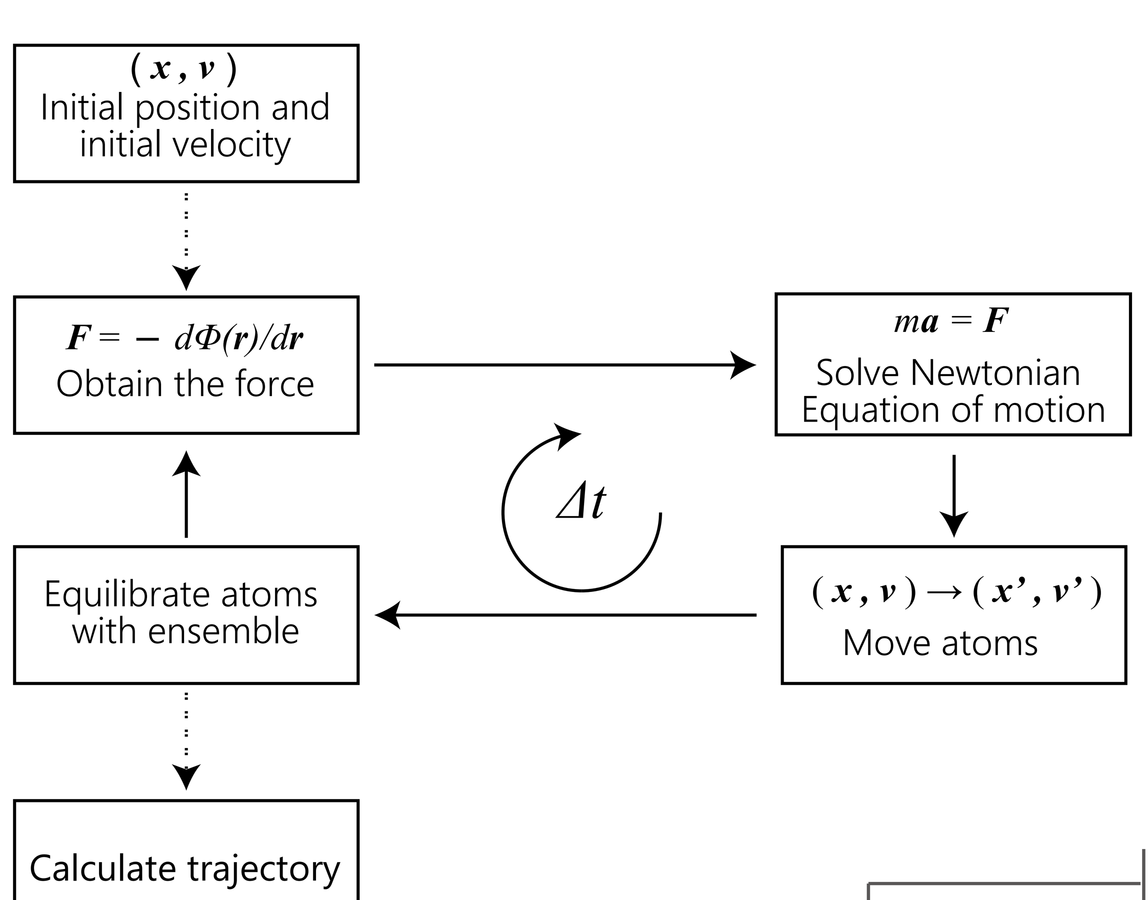
- In this study, we have used interaction potential including intramolecular and intermolecular potentials.

$$\phi = \sum_{ij}^{b} k_r (r - r_0)^2 \quad \text{Telescopic movement}$$

$$+ \sum_{ijk}^{a} k_\theta (\theta - \theta_0)^2 \quad \text{Bending movement}$$

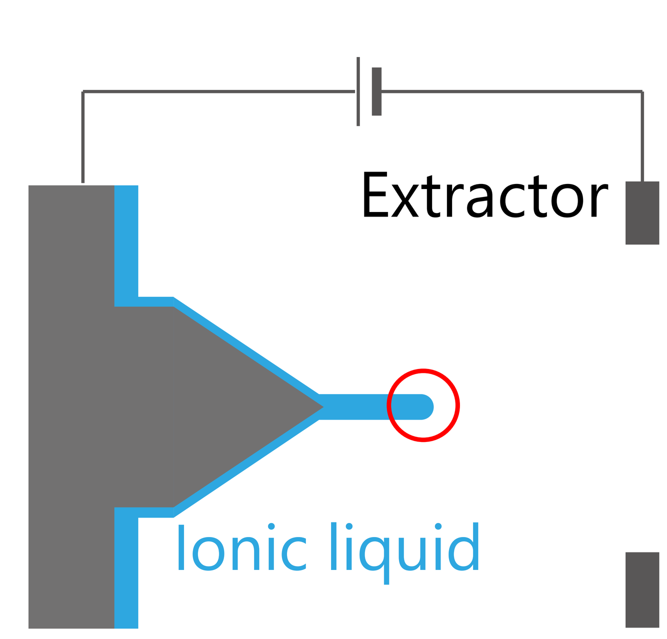
$$+ \sum_{ijkl}^{d} \sum_{m=1}^{4} \frac{k_{m,ijk}}{2} \left[1 + (-1)^m \cos(m\psi_{ijkl})\right] \quad \text{Twisting movement}$$

$$+ \sum_{i} \sum_{i \neq j} s_{ij} \left(4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] + \frac{1}{4\pi\varepsilon_0}\frac{q_i q_j}{r_{ij}}\right) \quad \text{Lennard-Jones potential and Coulomb potential}$$



Calculation conditions

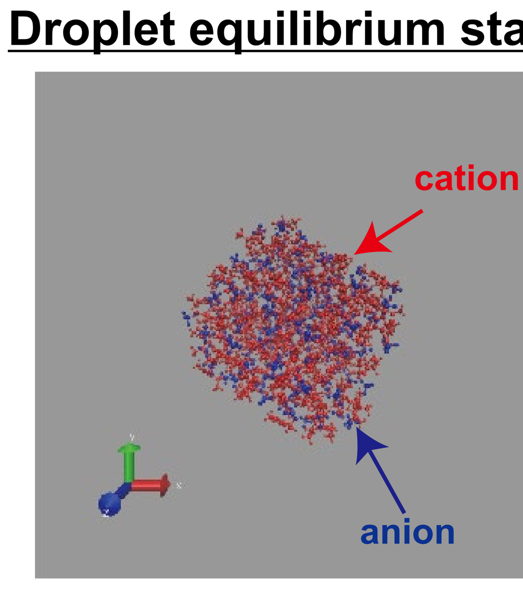
Ionic liquid	EMI-BF$_4$
Time step	0.5 fs
Number of molecules	125
Cutoff distance	12 Å (LJ)
Electric field	1.5 V/nm



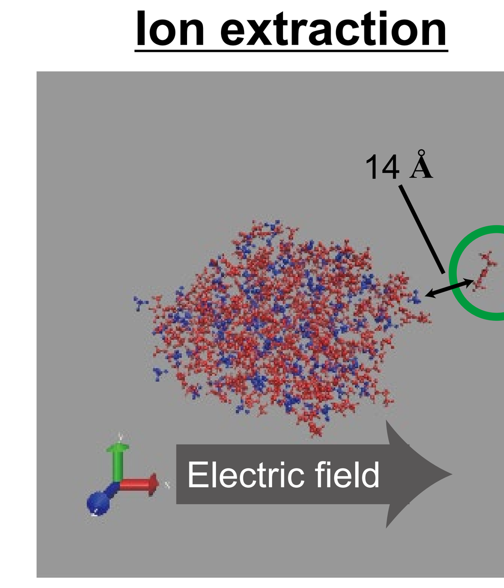
- We have used 125 EMI-BF$_4$ molecules, which corresponds to a droplet of 4 nm in the red circle.

3. Results and Discussion

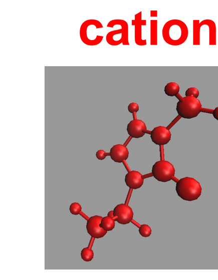
Droplet equilibrium state



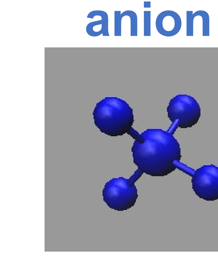
Ion extraction



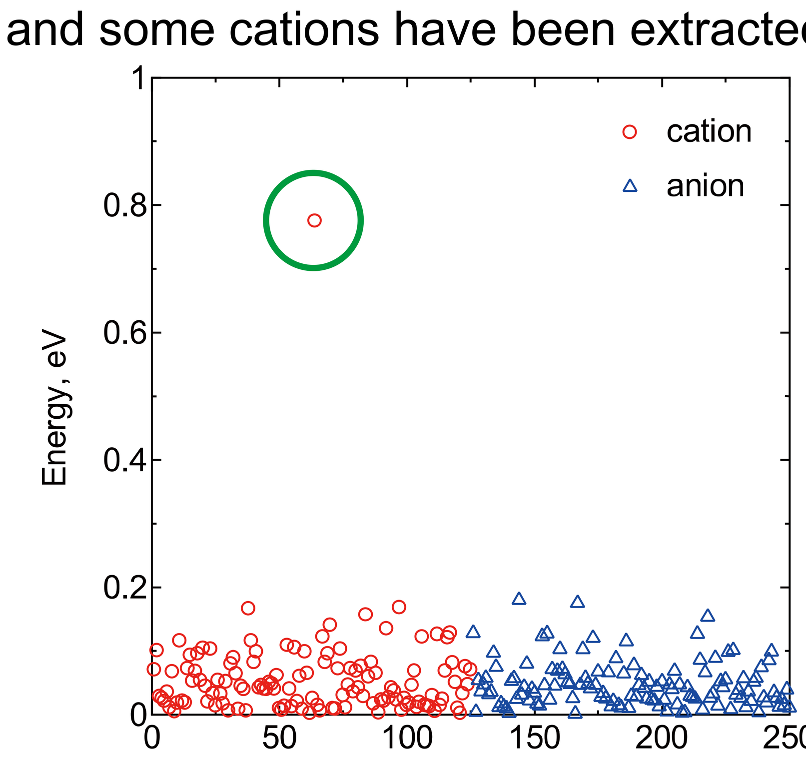
cation

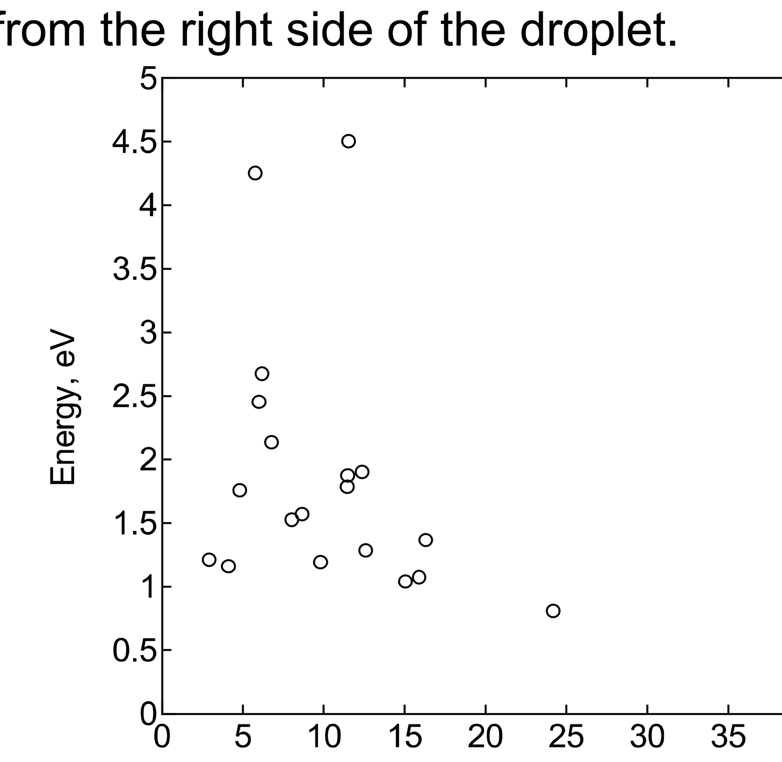


anion



- Red molecules are cations and blue molecules are anions.
- We have applied an uniform electric field along the *x*-axis direction, and some cations have been extracted from the right side of the droplet.



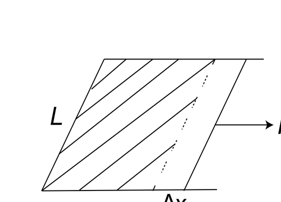


- The energy of the extracted ions were increasing.
- The lowest kinetic energy of the extracted ion was approximately 0.8 eV.
- Most extracted angles were 20° or less.

Validation of the kinetic energy

- When ions are extracted from a droplet of diameter L by Δx, the surface tension acting on the liquid is shown as

$$\gamma = \frac{W}{L\Delta x}.$$



- We used the table value and got the theoretical value 0.8-1.7 eV.
- The kinetic energy of 0.8 eV was suitable for the energy at the boundary where ions were extracted.

The value used in the calculation.

γ (experimental value)	5.03 × 10^{-2} N/m
L	20-40 Å
Δx	14 Å

4. Conclusion

- We have conducted molecular dynamics simulations of the ionic liquid in IELSTs and investigated the ion extraction mechanism.
- Under a uniform electric field, the minimum kinetic of the extracted ions was 0.8 eV and the extracted angles were less than 25°.
- We evaluated the kinetic energy by surface tension and confirmed that the kinetic energy obtained was in good agreement with that from the simple model.