Research On Sympathetic Cooling $^{113}Cd^{+}$-$^{174}Yb^{+}$ System By Molecular Dynamics Simulation

S. N. Miao, J. W. Zhang, N. C. Xin, L. M. Guo, H. X. Hu, W. X. Shi, L. J. Wang
State Key Laboratory of Precision Measurement
Department of Precision Instruments, Tsinghua University
Beijing 100084, P. R. China
E-mail: zhangjw@tsinghua.edu.cn

H. R. Qin, J. Z. Han, L. J. Wang
Department of Physics, Tsinghua University
Beijing 100084, P. R. China

***Abstract*—A microwave ion clock based on $^{113}Cd^{+}$ ions at Tsinghua University has been carried out for eleven years. To improve the performance of the ion clock with lower second-order Doppler frequency shift and suppressed Dick effect, a high-performance scheme for sympathetically cooling $^{113}Cd^{+}$ ions based on molecular dynamics simulation is reported.**

Keywords—molecular dynamics; microwave clocks; sympathetic cooling

I. INTRODUCTION

The laser cooling technology makes it possible to obtain cold ion ensembles at ultra-low temperature, which was widely used in quantum frequency standard[1], quantum information processing[2], and tests of fundamental physics in a variety of fields. However, lasers in most wavelength ranges can't be obtained due to the limit of technology, and only a small part of ions can be cooled by laser directly. For ions that can't be directly cooled by laser, sympathetic cooling by the long-range Coulomb interaction among ions has attracted a wide spread attention. In the sympathetic cooling scheme, the sympathetic-cooled (SC) ions' temperature is reduced close to the Doppler limit through Coulomb interactions with laser-cooled (LC) ions.

Since 2010, at Tsinghua University, our team has been committed to developing a microwave ion clock based on $^{113}Cd^{+}$ ions. So far, the frequency of the clock transition was obtained to be 15199862855.0192(10) Hz with a fraction uncertainty of 6.6×10^{-14}, and the frequency instability was measured to be $6.1 \times 10^{-13}\tau^{-1/2}$[3]. To reduce the uncertainty of the second-order Doppler shift (SODS) and the limitation arising from the Dick effect to short-term stabilities, we have been using $^{40}Ca^{+}$ ions as the coolant ions to sympathetically cool $^{113}Cd^{+}$ ions since 2019[4]. However, the $^{113}Cd^{+}$ ions locate far from the trap axial as a shell outside of the $^{40}Ca^{+}$ ions when the ions are laser cooled due to the big mass ratio of $m_{Cd^+}/m_{Ca^+} = 113/40$, which leads to a larger SODS due to the micromotion. If we use a kind of coolant ions with heavier mass than $^{113}Cd^{+}$ ions, more $^{113}Cd^{+}$ ions could locate close to the trap axial, which will bring smaller SODS than the one of the previous scheme.

In this paper, we propose to use $^{174}Yb^{+}$ ions as the coolant ions to sympathetically cool $^{113}Cd^{+}$ ions based on the molecular dynamics(MD) simulation[5], which is able to suppress the SODS while achieving sympathetic cooling of $^{113}Cd^{+}$ ions.

II. EXPERIMENT SETUP

In our experiment, both Cd^{+} and Yb^{+} ions are trapped in a linear Paul trap at the same time. The ion trap and the corresponding coordinates used in the experiment are shown in Fig. 1. The linear ion trap consists of four parallel stainless-steel cylindrical electrode rods in a quadrupole configuration, and each rod is segmented into three parts for three-dimensional(3D) trapping of ions. The length of the trapping part(B) and the remaining parts(A,C) of each electrode rod are $2z_0 = 40$ mm and $2z_e = 20$ mm, respectively. The diameter of each rod is 14.2 mm, and the minimum distance between the nodal line of the trap and the electrode surfaces is 6.2 mm.

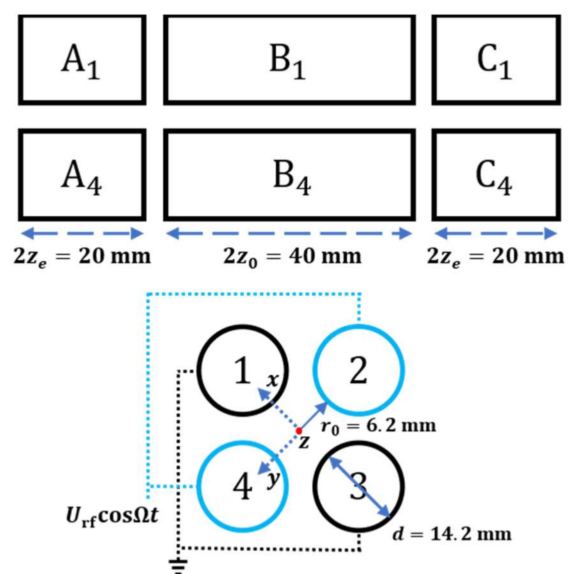

Fig. 1. Sketch of the linear Paul trap and RF potential.

The confinement of the ions in the radial plane is achieved by applying a radio frequency(RF) field $U_{rf}\cos\Omega t$ to one pair of diagonal electrode rods, and the other pair are grounded. The RF frequency is 2 MHz, and the amplitude U_{rf} can be adjusted in the range from 50 V to 1000 V. The confinement of the ions

978-1-6654-3935-0/21/$31.00 ©2021 IEEE

in the axial direction is achieved by applying direct current(DC) voltage U_{end} to the end parts of electrode rods.

It is well known that the motion of a single ion in the Paul trap can be described by the Mathieu equation[6]:

$$\frac{d^2r}{d\xi^2} + (a - 2q\cos 2\xi)r = 0.$$

When $(|a|,\ q^2) \ll 1$, the ion trajectory can be approximated as follows:

$$r(t) = r_s \cos(\omega_r t)\left[1 + \frac{q}{2}\cos(\Omega t)\right].$$

As can be seen, the motion of an ion in the trap can be described the secular motion with frequency ω_r plus the micromotion with frequency Ω. The energy of the secular motion can be deduced by laser cooling or sympathetic cooling, but the micromotion is driven by RF field, which can't be reduced. For an ion that locates outside the nodal line of the trap, the farther away from the nodal line, the greater the amplitude of the micromotion[7], which leads to larger SODS even if the ion is cooled to the Doppler limit temperature.

III. MD SIMULATION

The simulation model is built based on solving Newton's equation of motion[5] for all laser-cooled and sympathetically cooled ions as

$$\begin{aligned} m_i\ddot{r_i} &= F_i(r_{1,\dots,}r_{LC+SC}, v_{1,\dots,}v_{LC+SC}, t) \\ &= F_i^{\text{trap}} + F_i^{\text{Coulomb}} + F_i^{\text{stochastic}} + F_i^{\text{laser}}, \end{aligned}$$

where $i = 1,2, \dots, N_{\text{LC}} + N_{\text{SC}}$($N_{\text{LC}}$ and N_{SC} are the number of the laser-cooled and sympathetically cooled ions), m_i, r_i, v_i are the ion's mass, position and velocity, respectively. In our simulation model, there are four forces to be considered, and they are F_i^{trap}, F_i^{Coulomb}, $F_i^{\text{stochastic}}$ and F_i^{laser}. F_i^{trap} is the trapping potential force, which can be given by

$$F_i^{\text{trap}} = -Q_i\nabla\varphi(x, y, z, t),$$

where $\varphi(x, y, z, t)$ is the time-varying potential in the linear ion trap as

$$\begin{aligned} \varphi(x, y, z, t) &= \frac{U_{\text{rf}}}{2r_0^2}(x^2 - y^2)\cos(\Omega t) \\ &\quad + \frac{\kappa U_{\text{end}}}{2z_0^2}(2z^2 - x^2 - y^2). \end{aligned}$$

F_i^{Coulomb} is the Coulomb interaction force on ion i from remaining ions, which can be expressed as follows:

$$F_i^{\text{Coulomb}} = \frac{Q_i}{4\pi\varepsilon_0}\sum_{j\neq i}\frac{Q_j}{{r_{ij}}^2},$$

where r_{ij} is the distance between ions i and j, ε_0 is the vacuum permittivity. The stochastic force $F_i^{\text{stochastic}}$ represents all possible heating factors, for instance, RF heating, the imperfections of the ion trap, the collisions between the ions and the background gas molecules, etc. The laser cooling force F_i^{laser} can be considered as a linear viscous damping force plus a constant light pressure force in the direction of the cooling laser:

$$F_i^{\text{laser}} = -\alpha_i\dot{r_i} + F_i^{\text{lp}},$$

where α_i is the damping coefficient related to the laser power density and frequency detuning, F_i^{lp} is the laser radiation force related to the direction of propagation and power density of the laser.

The position, velocity and acceleration of each ion are updated with 'Leapfrog' integration algorithm[8]. Compared with the experiment, the information of all laser-cooled ions and sympathetically cooled ions can be obtained at any time based on the MD simulation, which is very useful for studying the evolution process and structural characteristics of the ion system[9,10].

IV. PRELIMINARY RESULTS AND DISCUSSION

The CCD image of the $^{113}Cd^+$-$^{174}Yb^+$ ion crystal is obtained from the simulation output, as shown in Fig. 2(a). The red dots and green dots represent Yb^+ ions and Cd^+ ions, respectively. The number of Yb^+ ions and Cd^+ ions are 512 and 256. After reaching equilibrium state, the secular energy per Cd^+ ion is about 12mK·3k$_B$/2, and the total energy per Cd^+ ion is about 0.71K·3k$_B$/2. Under the same simulation parameters, the $^{113}Cd^+$-$^{40}Ca^+$ ion crystal is obtained, as shown in Fig. 2(b). The red dots and green dots represent Ca^+ ions and Cd^+ ions, and the number of Ca^+ ions and Cd^+ ions are 512 and 256. In equilibrium state, the secular energy per Cd^+ ion is about 88mK·3k$_B$/2, and the total energy per Cd^+ ion is about 4.8K·3k$_B$/2. Based on the simulation results of these two sympathetic cooling schemes, the secular energy of Cd^+ ions is greatly reduced by sympathetic cooling and can be ignored compared with the micromotion energy. And both the secular energy and the micromotion energy of Cd^+ ions with Yb^+ ions as coolant are much lower than that with Ca^+ ions as coolant, which could has promising performance of microwave ion clocks with smaller SODS and suppressed Dick effect.

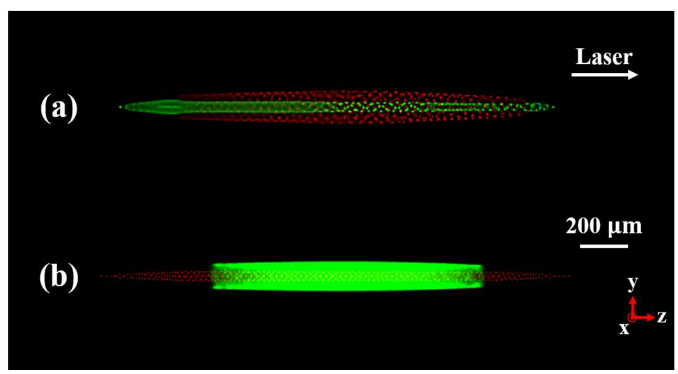

Fig. 2. (color online) Simulated CCD images of dual species ion system: (a) $^{113}Cd^+$-$^{174}Yb^+$ ion crystal, (b) $^{113}Cd^+$-$^{40}Ca^+$ ion crystal.

In equilibrium state, the temperature of SC ions is a little higher than that of LC ions due to RF heating, and the equilibrium temperature of SC ions is related to the number ratio between LC ions and SC ions. Fig. 3 shows the relationship between the equilibrium temperature of Cd^+ ions in the $^{113}Cd^+$-$^{174}Yb^+$ ion system and the number ratio of two types of ions. In the simulation experiment, the number of Cd^+ ions is fixed at 256. As the number of Yb^+ ions increases, the equilibrium temperature of Cd^+ ions gradually decreases, and the optimal number ratio is about 2. When the number ratio of Yb^+ ions and Cd^+ ions is greater than 2, the equilibrium temperature of Cd^+ ions remains basically unchanged. In the sympathetic cooling scheme, the optimal ion number ratio is of great significance for improving cooling efficiency and further improving the performance of the Cd^+ ion microwave clock.

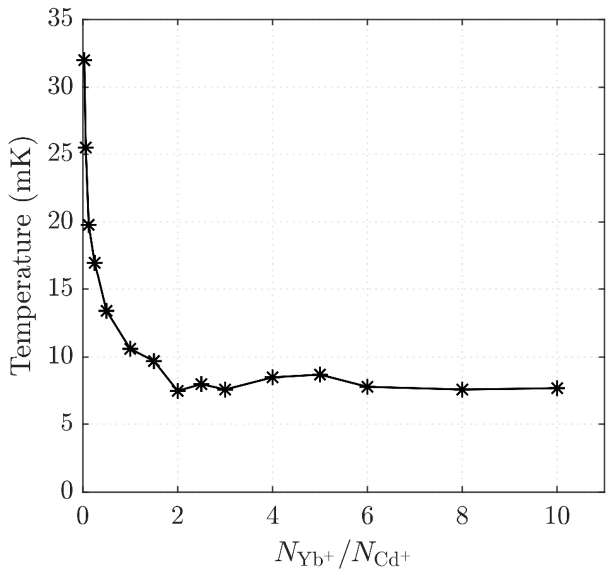

Fig. 3. The relationship between the equilibrium temperature of Cd^+ ions and the number ratio between Yb^+ ions and Cd^+ ions.

So far, limited by the hardware conditions, there are only a small number of ions in total in the MD simulation. In the near future, we will expand the total number of ions to the level of 10^5, which is the same order of magnitude as the number of ions in the experiment, and we believe that the simulation results will greatly assist the experiment. Therefore, these works are still undergoing.

Acknowledgment

We thank Y.N. Zuo and W. Liao for the greatest help on MD code programming.

References

[1] Huntemann, M. Okhapkin, B. Lipphardt, S. Weyers, Chr. Tamm, and E. Peik, "High-Accuracy Optical Clock Based on the Octupole Transition in $^{171}Yb^+$," Phys. Rev. Lett., vol. 108, no. 9, p. 090801, Feb. 2012.

[2] H. Häffner, C. F. Roos, and R. Blatt, "Quantum computing with trapped ions," Physics Reports, vol. 469, no. 4, pp. 155–203, Dec. 2008.

[3] K. Miao et al., "High accuracy measurement of the ground-state hyperfine splitting in a $^{113}Cd^+$ microwave clock," Opt Lett, vol. 40, no. 18, pp. 4249–4252, Sep. 2015.

[4] J. Z. Han et al., "Toward a high-performance transportable microwave frequency standard based on sympathetically cooled $^{113}Cd^+$ ions," Appl. Phys. Lett., vol. 118, no. 10, p. 101103, Mar. 2021.

[5] C. B. Zhang, D. Offenberg, B. Roth, M. A. Wilson, and S. Schiller, "Molecular-dynamics simulations of cold single-species and multispecies ion ensembles in a linear Paul trap," Phys. Rev. A, vol. 76, no. 1, p. 012719, Jul. 2007.

[6] W. Paul, O. Osberghaus, and E. Fischer, "Forschungsber. Wirtsch," Verkehrminist. Nordrhein-Westfalen, vol. 415, no. 1, 1958.

[7] D. J. Berkeland, J. D. Miller, J. C. Bergquist, W. M. Itano, and D. J. Wineland, "Minimization of ion micromotion in a Paul trap," Journal of Applied Physics, vol. 83, no. 10, pp. 5025–5033, Apr. 1998.

[8] R. P. Feynman, R. B. Leighton, and M. Sands, "The Feynman Lectures on Physics; Vol. I," American Journal of Physics, vol. 33, no. 9, pp. 750–752, Sep. 1965.

[9] L. Hornekær, N. Kjærgaard, A. M. Thommesen, and M. Drewsen, "Structural Properties of Two-Component Coulomb Crystals in Linear Paul Traps," Phys. Rev. Lett., vol. 86, no. 10, pp. 1994–1997, Mar. 2001.

[10] K. Okada, M. Wada, T. Takayanagi, S. Ohtani, and H. A. Schuessler, "Characterization of ion Coulomb crystals in a linear Paul trap," Phys. Rev. A, vol. 81, no. 1, p. 013420, Jan. 2010.