Dynamic Analysis of Two Rotating-Particles Collision Process by Molecular Dynamics Method

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Introduction

Whether the rotational motion of a particle involved in a collision process should be taken into account in a mathematical model is a matter of interested concerned. Dynamic analysis has been done without considering such the rotational motion [1], [2]. The purpose of this study is to take a basic knowledge of how much the rotational motion affects the size of a coalesced particle. A computer code is developed to examine the dynamics of two rotating-particles collision process. When the collision between the two particles takes place, it will lead to a coalesced process. The size distribution of coalesced particle is revealed from a microscopic point of view. Computer simulation suggested that the effect of the rotational motion is noticeable in the early stage of the particle growth process.

Calculation Model

First thing, we need to make a computer program based on the Molecular Dynamics method. For simplicity of the mathematical model, the interaction between the two molecules is assumed to be described by the Lennard-Jones (12 - 6) potential function. A model particle is composed of 1000 UF_6 molecules, the size of which is in the order of nanometer and its temperature is about 150 K. Three types of rotational mode are considered, there are a clockwise-clockwise, a clockwise-counterclockwise on an X-axis and a clockwise-clockwise on a Y-axis. Figure 1 shows the initial configuration of a two-particle collision system. Rotating-particle is forced into a head-on collision with the velocity of 3 m/s each.

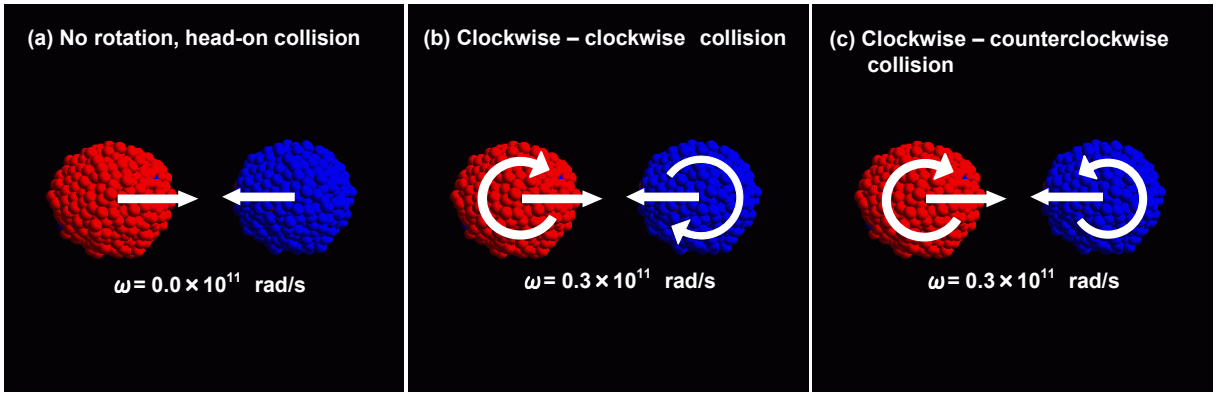

Figure 1. Initial configuration of a head-on collision system for computer simulation

Simulation Results

If the model particle rotates on its axis at a constant angular velocity, a shape deformation like an ellipsoid would occur to a certain extent. In relation to the particle's rotation, there exists a critical angular velocity, at which a breakup just begins [3]. As far as the model particle has less than the critical angular velocity, it will keep its shape almost unchanged. Let's take an example of the head-on collision between the two rotating particles with the angular velocity of 0.3×10^{11} rad/s each. After the collision took place they go into the coalescence process. Eventually the coalesced particle is expected to form into a spherical shape. Dynamics of the coalescence process is shown in Fig.2 for the elapsed time of 4000 ps. During the coalescence process, a few UF_6 molecules are emitted from its surface to cool itself off. Therefore the size of the coalesced particle will become

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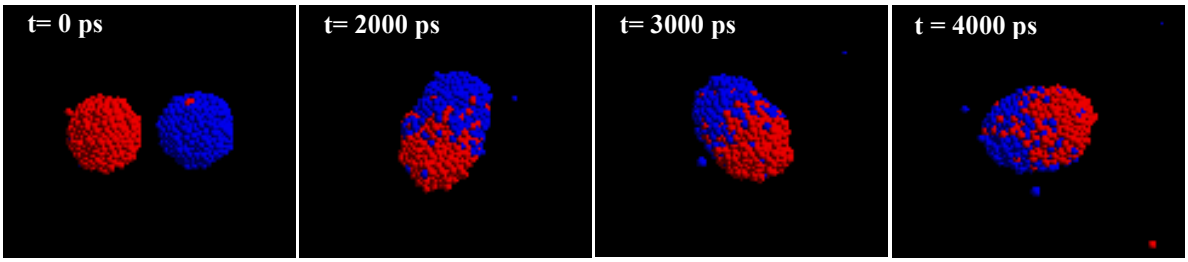
different depending on the number of the emitted UF_6 molecules. Figure 3 shows the effect of the rotational motion on the particle size distribution.



Figuer.2 Dynamics of the coalescence process of the two-rotating particle, clockwise-clockwise collision

We can see there is no such the case that the coalesced particle is made up of 2000 UF_6 molecules. That is they never coalesce without emitting UF_6 molecules. If an i-cluster collided with a j-cluster, there is a little possibility of producing (i+j) cluster. Computer simulation showed, as a general tendency, that the smaller the size of the rotating particle, the higher the emitting rate of UF_6 molecules is. Finally, the emitting of UF_6 molecules will cause a change of the particle's potential energy, but it could not lead to the particle breakup process.

Conclusions

The findings obtained here are very important when we make the mathematical model in the early stage of the particle growth process. The rotational motion itself is not much involved in the breakup process as long as the particle rotates within the critical angular velocity. We will plan to carry out computer simulation under some different conditions from now on.

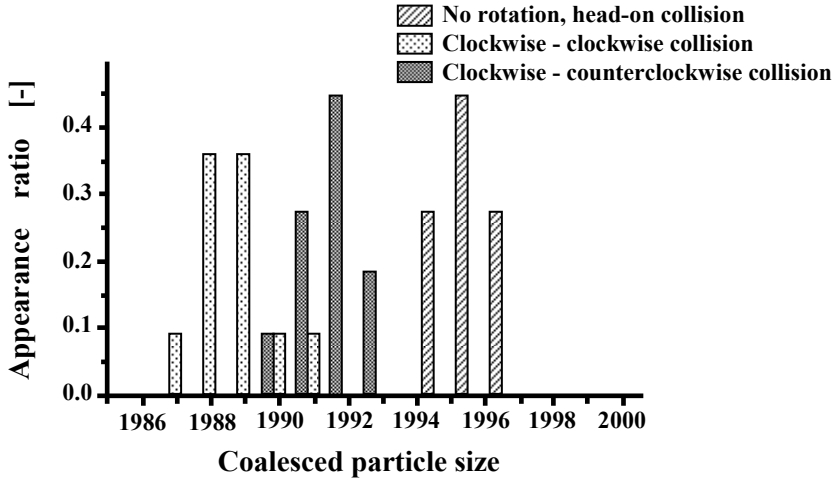


Figure 3. Size distribution of the coalesced particle formed after the two-rotating particle collision

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References

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