Formation of Nuclear "Pasta" in Supernovae

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In supernova cores, nuclear "pasta" phases such as a triangular lattice of rodlike nuclei and layered structure of slablike nuclei are considered to exist. However, it is still unclear whether or not they are actually formed in collapsing supernova cores. Using *ab initio* simulations called quantum molecular dynamics, here we solve this problem by demonstrating that a lattice of rodlike nuclei is formed from a bcc lattice by compression. We also find that, in the transition process, the system undergoes a zigzag configuration of elongated nuclei, which are formed by a fusion of two original spherical nuclei.

The mechanism of collapse driven supernova explosions [1] has been a long-standing mystery [2]. Matter in supernova cores is also yet to be understood and these issues are closely connected. In the initial stage of the explosions, the collapsing iron core experiences an adiabatic compression, which leads to an increase of the central density from $\sim 10^9$ g cm^{-3} to around the normal nuclear density $\sim 3 \times 10^{14}$ g cm^{-3} (corresponding to the nucleon number density $\rho_0 = 0.165$ fm^{-3}) just before the star rebounds. Thereby, the Coulomb repulsion between protons in nuclei, which tends to make a nucleus deform, becomes comparable to the surface tension of the nuclei, which favors a spherical nucleus. The pasta phases (phases consisting of "spaghetti-like" columnar nuclei and of "lasagnalike" planar nuclei, etc.) [3–5] are thus expected to be formed in the inner cores during the collapse of stars and amount to more than 20% of the total mass of the cores just before the bounce [6]. Since the coherent scattering of neutrinos is very different between pasta nuclei and spherical ones [7,8], pasta phases can have a significant influence on the dynamics of explosions [6,8]. Thus there is a growing interest in pasta phases [9].

However, the above speculation that the pasta phases are formed in collapsing cores is based on phase diagrams of the equilibrium state (e.g., Refs. [10–14] for nonzero temperatures) or static and perturbative calculations [15,16]. Since the formation of the pasta phases from a bcc lattice of spherical nuclei is accompanied by dynamical and drastic changes of the nuclear structure, the fundamental question whether or not the pasta phases are formed in supernova cores is still open, and an *ab initio* approach is called for. In the present work, we answer this question using called the quantum molecular dynamics (QMD) [17,18]. QMD can properly incorporate the thermal fluctuations and is a

powerful and suitable approach [19] to describe the deformation of nuclei in the present problem as has been exploited for studying the equilibrium phase diagram [12,20] and the transition dynamics between the pasta phases [21].

We use the QMD Hamiltonian of Ref. [18] with the standard medium-equation-of-state parameter set [22]. In our simulations, we consider a system with protons, neutrons, and charge-neutralizing electrons in a cubic box with periodic boundary condition. The electrons are relativistic and degenerate, and can be well approximated as a uniform background [15,23]. We calculate the Coulomb interaction by the Ewald sum. Our simulations are carried out for the proton fraction $x \simeq 0.39$ and 0.49 using different initial conditions of the bcc lattice. In the following, we focus on the results for $x \simeq 0.39$ (the qualitative results are the same for $x \simeq 0.49$).

The initial condition of $x \simeq 0.39$ is obtained in the following way. We first prepare an isolated nucleus of ^{208}Pb at zero temperature and make a unit cell of the bcc lattice by setting two copies of the nuclei in a box with the periodic boundary condition. Using the Nosé-Hoover thermostat for momentum-dependent potentials [12], we then equilibrate this sample at the temperature $T = 1$ MeV. We combine eight replicas of this bcc unit cell to make a sample of the total number of nucleons $N = 3328$ (with 1312 protons and 2016 neutrons) at the nucleon number density $\rho = 0.15\rho_0$ (the box size $L = 51.23$ fm) and equilibrate at $T = 1$ MeV for $\simeq 7800$ fm/c using the Nosé-Hoover thermostat and further relax for $\simeq 4100$ fm/c without the thermostat. Equilibrating this sample at different temperatures, we also prepare initial conditions for various temperatures.

We simulate the compression of the bcc phase of spherical nuclei in the collapse. Starting from the above initial

conditions, we increase the density by changing the box size L (the particle positions are rescaled at the same time). Here the average rate of the compression is $\lesssim \mathcal{O}(10^{-6})\rho_0/(\text{fm}/c)$ yielding the time scale of $\gtrsim 10^5$ fm/c to reach the typical density region of the phase with rodlike nuclei. This is much larger than the time scale of the change of nuclear shape (e.g., ~ 1000 fm/c for nuclear fission) and thus the dynamics observed in our simulation would be determined by the intrinsic physical properties of the system, not by the density change applied externally. We perform adiabatic compression and isothermal compression at various temperatures [24]. In all the cases, we observe the formation of rodlike nuclei; here we show some typical examples in which we obtain a clear lattice structure of the rodlike nuclei.

Figure 1 shows the snapshots of the formation process of the pasta phase in adiabatic compression. Here, we start
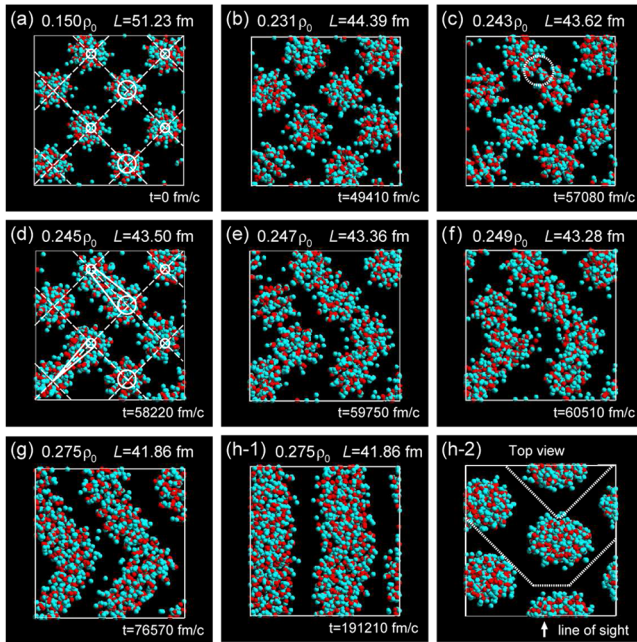

FIG. 1 (color online). Snapshots (two-dimensional projection) of the transition process from the bcc lattice of spherical nuclei to the pasta phase with rodlike nuclei. The red particles show protons and the green ones neutrons. In panels (a)–(g) and (h-1), nucleons in a limited region relevant for the two rodlike nuclei in the final state (h) [surrounded by the dotted lines in panel (h-2)] corresponding to eight nuclei in the initial condition (a) are shown for visibility. The vertices of the dashed lines in panels (a) and (d) show the equilibrium positions of nuclei in the bcc lattice and their positions in the direction of the line of sight are indicated by the size of the circles: vertices with a large circle, with a small circle, and those without a circle are in the first, second, and third lattice plane, respectively. The dotted circle in panel (c) show the first pair of nuclei start to touch. The solid lines in panel (d) represent the direction of the two elongated nuclei: they take zigzag configuration. In the final state [(h-1) and (h-2)], almost perfect triangular lattice of rodlike nuclei is obtained. The box sizes are rescaled to be equal in the figures.

from the initial condition of $x = 0.39$ and $T = 0.25$ MeV ($t = 0$ fm/c). At $t \simeq 57\,080$ fm/c and $\rho \simeq 0.243\rho_0$ [Fig. 1(c)], the first pair of two nearest-neighbor nuclei start to touch and fuse (dotted circle), and then form an elongated nucleus [see, e.g., Fig. 1(d)]. After multiple pairs of nuclei become such elongated nuclei, we observe zigzag structure as shown in Fig. 1(d). These elongated nuclei start to stick together at $t \simeq 59\,000$ fm/c and $\rho = 0.246\rho_0$, and all the nuclei fuse to form rodlike nuclei at $t \lesssim 72\,700$ fm/c and $\rho \lesssim 0.267\rho_0$. At $t = 76\,570$ fm/c and $\rho = 0.275\rho_0$, we stop the compression ($T \simeq 0.5$ MeV in this stage). We then relax the system microcanonically for $65\,510$ fm/c and further relax at $T = 1$ MeV for $\simeq 10\,000$ fm/c (after that we take back the temperature to $\simeq 0.5$ MeV and relax for $\simeq 20\,000$ fm/c; for the increase and decrease of the temperature between 0.5 and 1 MeV, we take $\simeq 5000$ and $\simeq 15\,000$ fm/c, respectively). Finally, we obtain a triangular lattice of rodlike nuclei [Figs. 1h-1 and 1h-2]. The remarkable point is that, in the middle of the transition process, a pair of spherical nuclei get closer to fuse in a way such that the resulting elongated nuclei take a zigzag configuration (hereafter, we call it "zigzag pairing") and they further connect to form wavy rodlike nuclei. This feature is observed in all the other cases in which we obtain a clear lattice structure of rodlike nuclei (among them, the highest temperature case is the adiabatic compression from $T = 1.5$ MeV), and the above scenario of the transition process is qualitatively the same also for those cases. It is very different from a generally accepted picture (see, e.g., p. 462 of Ref. [15]) that all the nuclei elongate in the same direction along the global axis of the resulting rodlike nuclei and they join up to form straight rodlike nuclei.

It has been regarded so far that the formation of the pasta phases in supernova cores is triggered by the fission instability with respect to the quadrupolar deformation of spherical nuclei [15]. To examine this point, we investigate the variance of the radius of each nuclei over the solid angle and the area-averaged mean curvature of the nuclear surface; neither of these quantities show a significant increase throughout the compression process until the nuclei start to touch [see also Fig. 1(b)]. This means that, before nuclei deform to be elongated due to the fission instability, they stick together keeping their spherical shape. This is consistent with the result of Ref. [25] (see also Ref. [26]), which shows that, within an incompressible liquid-drop model, the condition for the fission instability is not satisfied if one takes account of the background electrons.

To understand the mechanism which triggers the formation of the pasta phases, we calculate the distance r_{nn} between centers of mass (for protons) of nearest-neighbor nuclei in the compression process of our simulations [27]. Figure 2 shows the mean value $\langle r_{nn} \rangle$ and the standard deviation Δr_{nn} of r_{nn} calculated for 16 nuclei in the simulation box. Let us first focus on the result obtained for the
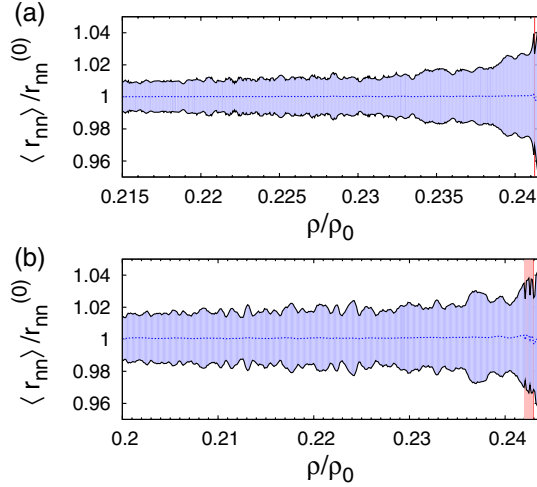
FIG. 2 (color online).   Distance r_{nn} between centers of mass of nearest-neighbor nuclei in the compression process. The blue line shows the mean value $\langle r_{nn} \rangle$ and the blue filled region shows the standard deviation Δr_{nn} of r_{nn} normalized by $r_{nn}^{(0)}$ (a value of r_{nn} for a perfect bcc lattice without displacement of nuclei). Panel (a) is for the isothermal compression at $T = 0$ MeV and panel (b) is for the adiabatic compression starting from $T = 0.25$ MeV. The first pair of nuclei touch at a density in the red filled region (corresponding to $r_{nn}^{(0)} \simeq 18.9$ fm for both cases) whose width shows its uncertainty.

isothermal compression at $T = 0$ MeV [Fig. 2(a)], where we can see a clear signature due to the absence of thermal fluctuations. We note that there is a significant increase of Δr_{nn} just before the nuclei start to connect. This shows that, before pairs of nuclei touch, nuclei displace from the equilibrium position of the bcc lattice and the bcc structure is spontaneously broken. As a result, each pair of nuclei approach to fuse and then form an elongated nuclei arranged in a zigzag configuration. At nonzero temperatures, thermal fluctuation smears the above signature and it would also assist triggering the formation of the pasta phases; however even in the case of the adiabatic compression starting at $T = 0.25$ MeV, we can still see a significant increase of Δr_{nn} just before the nuclei touch and fuse [Fig. 2(b)].

Using a simplified model, we now examine our results of the QMD simulations. When nearest-neighbor nuclei are so close that the tails of their density profile overlap with each other, net attractive interaction between these nuclei starts to act due to the interaction between nucleons in different nuclei in the overlapping surface region. We consider that this attraction between nuclei leads to the spontaneous breaking of the bcc structure. In order to examine this hypothesis, we consider a minimal model in which each nucleus is treated as a point charged particle interacting through the Coulomb potential and the potential of the Woods-Saxon form: $V(r) = V_0\{1 + \exp[(r - R)/a]\}^{-1}$, which describes the finite size of nuclei and models the internuclear attraction when the nearest-

neighbor nuclei start to touch. Since nuclei start to connect before they are deformed, it is reasonable to treat a nucleus as a sphere and incorporate only its center-of-mass degree of freedom. Parameters R and a represent the interaction radius of a nucleus and range of the effective nuclear forces, respectively, and we take $V_0 = -11.5$ MeV, $R = 17$ fm, and $a = 0.5$ fm [28]. With this model, we carry out the isothermal (keeping the system cool at $T < 0.01$ MeV by the frictional relaxation method throughout the simulation; this small but nonzero temperature is sufficient for symmetry breaking) compression of the bcc lattice of 128 nuclei of ^{208}Pb, which corresponds to 8 times larger system than that of the QMD simulations. In Fig. 3 we show the snapshots of this simulation. Here we compress from $0.221\rho_0$ ($L = 90.00$ fm) at a rate of $\dot{\rho} < \mathcal{O}(10^{-6})\rho_0/(\text{fm}/c)$. At $0.246\rho_0$ ($L = 86.91$ fm) the first pair of nuclei starts to get closer [Fig. 3(b)] and then we stop the compression and relax the system. We observe zigzag pairing around the first pair [Fig. 3(c)] and finally we obtain a zigzag structure [Fig. 3(d)]. This supports that the zigzag structures observed in the QMD simulations are not caused by a finite size effect of the simulation box.

In conclusion, we have shown that an ordered structure of rodlike nuclei can be formed by compressing a bcc

(a) L=90.00 fm, t=0 fm/c   (b) L=86.91 fm, t=251810 fm/c

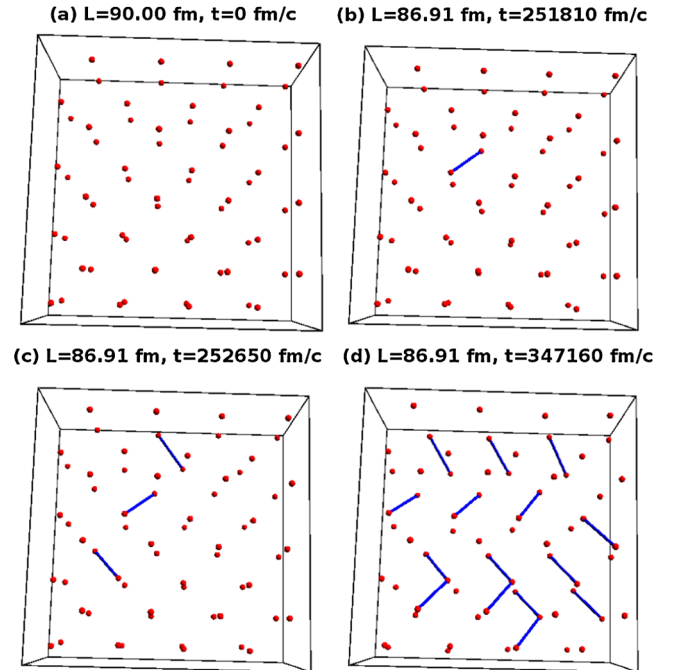(c) L=86.91 fm, t=252650 fm/c   (d) L=86.91 fm, t=347160 fm/c

FIG. 3 (color online).   Snapshots of the transition process in the simulation of isothermal compression at $T < 0.01$ MeV using the simplified model. Starting from the bcc lattice of nuclei (a), the first pairing (b), zigzag pairing around the first pair (c), and finally a zigzag structure (d) are observed. The red particles show the centers of mass of nuclei and the nuclei within the distance less than $0.89 r_{nn}^{(0)}$ are connected by a blue line. Nuclei and connections within only two lattice planes normal to the line of sight are shown.

lattice of spherical nuclei. Our result establishes that the pasta phases can be formed in collapsing supernova cores. Unlike a generally accepted conjecture, we have observed that nuclei start to connect before they deform due to the fission instability. This spontaneous breaking of the bcc structure is due to an attraction between nuclei caused by the overlap of the tails of nucleon distribution of neighboring nuclei. We have also discovered that, in the transition process, the system takes a zigzag configuration of elongated nuclei, which are formed by a fusion of original two spherical nuclei. Since a drastic change of the neutrino transport in the pasta phases pointed out in Ref. [7] has been already shown [8] (see also Ref. [6]), it is very interesting to perform core collapse simulations incorporating this effect as the next step.

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[28] In the relevant range of $r_{nn} \gtrsim 16$ fm [cf. $r_{nn}^{(0)} = 18.82$ fm at the highest density in this simulation corresponding to Figs. 3(b)–3(d)], this parameter set well reproduces the qualitative behavior of the potential between two nuclei of $Z = 82$ and $A = 208$ estimated by using the experimentally determined nucleon density distribution and mean-field potential of the Woods-Saxon form.
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