

Simulation of Transitions between “Pasta” Phases in Dense Matter

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Calculations of equilibrium properties of dense matter predict that at subnuclear densities nuclei can be rodlike or slablike. To investigate whether transitions between phases with nonspherical nuclei can occur during the collapse of a star, we perform quantum molecular dynamic simulations of the compression of dense matter. We have succeeded in simulating the transitions between rodlike and slablike nuclei and between slablike nuclei and cylindrical bubbles. Our results strongly suggest that nonspherical nuclei can be formed in the inner cores of collapsing stars.

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In ordinary matter, atomic nuclei are roughly spherical because, in the liquid drop picture of the nucleus, effects of the nuclear surface tension are greater than those of the Coulomb forces. When the density of matter approaches that of atomic nuclei, calculations predict that, in equilibrium state, the nuclei will adopt different shapes, such as cylinders, slabs, etc. These phases with nonspherical nuclei are often referred to as “pasta” phases [1,2].

In the initial stage of the supernova explosions, matter in the collapsing iron cores experiences an adiabatic compression, which leads to an increase of the density in the central region from $\sim 10^9 \text{ g cm}^{-3}$ to around the normal nuclear density $\rho_0 = 0.165 \text{ fm}^{-3}$ just before the star rebounds; the temperature there reaches the order of 1 MeV. The pasta phases are thus expected to be formed in the inner cores during the collapse of stars. However, such a speculation is based on phase diagrams of the equilibrium state (e.g., Refs. [3,4] for finite temperatures) or static and perturbative calculations [5,6]. It is still unclear whether the pasta phases can be formed and the transitions between them can be realized during the collapse, which lasts less than a second. Because of the drastic changes of nuclear shape that occur under nonequilibrium conditions, this problem is more difficult than the realization of the pasta phases by cooling at constant density, as demonstrated in Ref. [7], and an *ab initio* approach is called for.

In the present Letter, we solve the problem about the transitions between pasta phases using a dynamical framework for nucleon many-body systems called the quantum molecular dynamics (QMD) [8]. QMD is a suitable approach to describe thermal fluctuations and is efficient enough to treat large systems consisting of several nuclei. Furthermore, at the relevant temperatures of several MeV, shell effects, which cannot be described by QMD, are less important because they are washed out by thermal fluctuations.

The pasta phases have recently begun to attract the attention of researchers (see, e.g., Ref. [9], and references therein). The mechanism of the collapse-driven supernova explosion has been a central mystery in astrophysics for almost half a century. Previous studies suggest that the revival of the shock wave by neutrino heating is a crucial process. As has been pointed out in Refs. [7,10] and elaborated in Refs. [11,12], the existence of the pasta phases instead of uniform nuclear matter increases the neutrino opacity of matter in the inner core significantly [13] due to the neutrino coherent scattering by nuclei [14,15]; this affects the total energy transferred to the shocked matter. Thus the pasta phases could play an important role in the future study of supernova explosions.

In the present study, we use a nuclear force given by a QMD Hamiltonian with the medium–equation-of-state (EOS) parameter set in Ref. [16]. This Hamiltonian contains the momentum-dependent “Pauli potential,” which reproduces the effects of the Pauli principle phenomenologically. Parameters in the other terms of the Hamiltonian are determined to reproduce the saturation properties and the properties of finite nuclei in the ground state, especially of heavier ones relevant to the present study [16]. It is also confirmed that a QMD Hamiltonian close to the present model provides a good description of nuclear reactions including the low energy region (several MeV per nucleon) [17], which would be important for the present case.

Using the above QMD Hamiltonian, we perform simulations of symmetric nuclear matter with 16 384 nucleons in a cubic box with periodic boundary condition (see Ref. [12] for other cases). The system contains equal numbers of protons (and neutrons) with spin-up and spin-down. The relativistic degenerate electrons which ensure charge neutrality are treated as a uniform background because, at subnuclear densities, the effect of the electron screening is small [5,18]. The Coulomb energy, taking

account of the Gaussian charge distribution of the proton wave packets, is calculated by the Ewald method. The temperature T is measured by the effective kinetic temperature for momentum-dependent potentials, which is consistent with the temperature in the Boltzmann statistics [7]. The QMD equations of motion are integrated by the fourth-order Gear predictor-corrector method with a multiple time step algorithm. Integration time steps Δt are adaptive in the range of $\Delta t < 0.1\text{--}0.2$ fm/c.

As the initial condition, we use samples of the columnar phase and of the lamellar phase of 16 384-nucleon system at $T \approx 1$ MeV obtained in Ref. [4]. In preparing them, we first combine eight replicated 2048-nucleon samples in the ground state ($T \approx 0$ MeV; nucleon number density $\rho = 0.225\rho_0$ for the phase with rodlike nuclei and $0.4\rho_0$ for the case of slablike nuclei) into a 16 384-nucleon sample, and then put random noise on the positions and the momenta of nucleons up to 0.1 fm and 1 MeV/c, respectively. We equilibrate the sample at $T = 1$ MeV for $\sim 4000\text{--}5000$ fm/c using the Nosé-Hoover thermostat for momentum-dependent potentials [4]. We further relax the sample for ~ 5000 fm/c without the thermostat.

Starting from the above sample, we simulate the adiabatic compression. In the case starting from the phase with rodlike nuclei [slablike nuclei], the density is increased by $2 \times 10^{-4}\rho_0$ [$1 \times 10^{-4}\rho_0$] every 100 steps by changing the box size (the particle positions are rescaled at the same time). The average rate of change for the density is $\approx 1.3 \times 10^{-5}\rho_0/(\text{fm}/c)$ [$\approx 7.1 \times 10^{-6}\rho_0/(\text{fm}/c)$]; this rate ensures the adiabaticity of the simulated compression process with respect to the change of nuclear structure [19]. Finally, we relax the compressed sample at $\rho = 0.405\rho_0$ [$0.490\rho_0$]. These final densities are those of the phase with slablike nuclei [cylindrical bubbles] in the equilibrium phase diagram at $T \approx 1$ MeV [4].

The resulting time evolution of the nucleon distribution is shown in Figs. 1 and 2. Starting from the phase with rodlike nuclei [Fig. 1(a); $\rho = 0.225\rho_0$ (volume fraction of nuclear matter region $u = 0.20\text{--}0.22$ [20]) at time $t = 0$], the phase with a one-dimensional layered lattice of slablike nuclei is formed [Fig. 1(i); $\rho = 0.405\rho_0$ ($u = 0.41\text{--}0.45$) at $t = 17720$ fm/c]. During the compression, the temperature increases gradually up to ≈ 1.35 MeV in the final state. We note that, in the process of the compression, the phase with rodlike nuclei persists as a metastable state, and moreover, until nuclei begin to touch and fuse they are not elongated along the plane of the final slabs [see Fig. 1(b)]. This shows that the transition from the phase with rodlike nuclei to the slablike nuclei is not triggered by the fission instability. This result is consistent with a previous study, which shows the stability of the rodlike nuclei against a small quadrupolar deformation of the cross section [6]. When the internuclear spacing becomes small enough and once some pair of neighboring rodlike nuclei touch due to thermal fluctuations, they fuse [see the lower two nuclei in the middle column in Figs. 1(c) and 1(d); $u = 0.27\text{--}0.30$ at $t = 6050$ fm/c]. Like a chain reaction, such

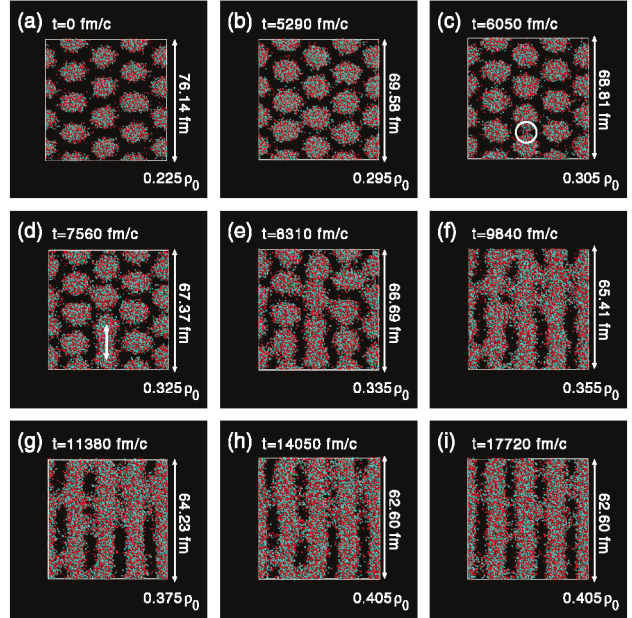


FIG. 1 (color). Snapshots of the transition process from the phase with rodlike nuclei to the phase with slablike nuclei (the whole simulation box is shown). The red particles show protons and the green ones neutrons. After neighboring nuclei touch, as shown by the circle in (c), the “compound nucleus” elongates along the arrow in (d). The box size is rescaled to be equal in this figure.

connected pairs of rodlike nuclei further touch and fuse with neighboring nuclei in the same lattice plane [see Figs. 1(e) and 1(f)]. Each fusion process in the chain reaction proceeds on a time scale of order 10^2 fm/c, which is much shorter than the time scale of the density change [19].

The transition from the phase with slablike nuclei to the phase with cylindrical holes is shown in Fig. 2 ($u = 0.42\text{--}0.45$ and $0.55\text{--}0.59$ at $t = 0$ and $27\,370$ fm/c). When the internuclear spacing decreases enough, neighboring slablike nuclei touch due to the thermal fluctuation as in the above case. Once nuclei begin to touch ($u = 0.49\text{--}0.52$ at $t = 8460$ fm/c), bridges between the slabs are formed at many places on a time scale (of order 100 fm/c) much shorter than that of the compression [cf. Figs. 2(c) and 2(d)]. After that the bridges cross the slabs nearly orthogonally for a while, which makes hollow regions on a square lattice rather than the final triangular one. Nucleons in the slabs continuously flow into the bridges, which become wider and merge together to form cylindrical holes. Afterwards, the connecting regions consisting of the merged bridges move gradually, and the cylindrical holes relax to form a triangular lattice. The final temperature in this case is ≈ 1.3 MeV.

Let us now investigate the detailed time evolution of the nuclear structure. The integral mean curvature and the Euler characteristic (see, e.g., Ref. [21]) are powerful tools for this purpose. Suppose there is a set of regions R , where the density is higher than a threshold density ρ_{th} . The integral mean curvature and the Euler characteristic for

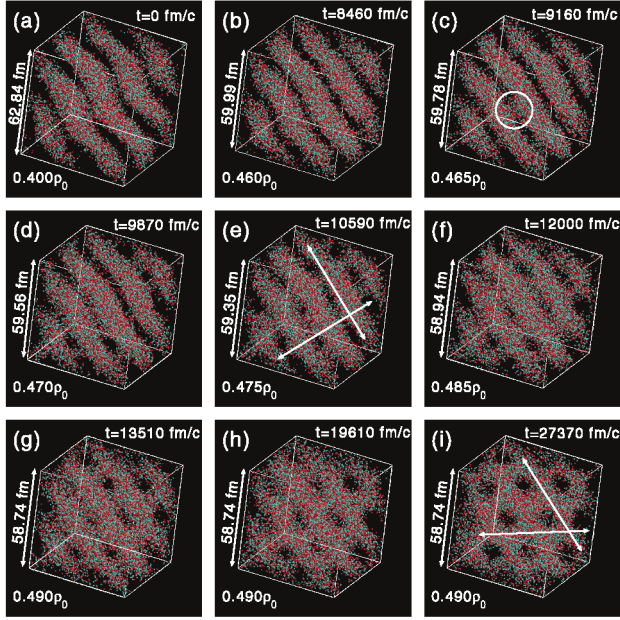


FIG. 2 (color). The same as Fig. 1 for the transition from the phase with slablike nuclei to the phase with cylindrical holes (the box size is not rescaled in this figure). After the slablike nuclei begin to touch [see the circle in (c)], the bridges first cross them almost orthogonally, as shown by the arrows in (e). Then the cylindrical holes are formed and they relax into a triangular lattice, as shown by the arrows in (i).

the surface of this region ∂R are defined as surface integrals of the mean curvature H and the Gaussian curvature G , respectively; i.e., $\int_{\partial R} H dA$ and $\chi \equiv \frac{1}{2\pi} \int_{\partial R} G dA$, where dA is the area element of the surface of R . The topological quantity $\chi = (\text{number of isolated regions}) - (\text{number of tunnels}) + (\text{number of cavities})$ [22]. We calculate these quantities using the density field of nucleons on 128^3 grid points (see Ref. [7] for detailed procedures).

In Figs. 3(a) and 3(b), the quantities $\int_{\partial R} H dA$ and χ calculated for each nucleon distribution in Fig. 1 are shown as functions of ρ_{th} . In this case, the initial condition is the phase with rodlike nuclei, whose structure is well characterized by the plateau of $\int_{\partial R} H dA \approx 4000$ fm [see the red curve in Fig. 3(a)]. The slablike nuclei in the final state, on the other hand, are characterized by $\int_{\partial R} H dA \approx 0$ fm, corresponding to the plateau of the gray curve in Fig. 3(a).

The behavior of χ clearly shows that the rodlike nuclei begin to touch between $t = 5290$ and 6050 fm/c, when the plateau value of χ starts to deviate from zero, characterizing the rodlike nuclei, to negative values, characterizing the multiply connected structures such as sponges. We note that before the nuclei touch the change in $\int_{\partial R} H dA$ is small except for lower values of $\rho_{\text{th}} \lesssim 0.1\rho_0$. This reflects the facts that the phase with rodlike nuclei persists as a metastable state and that the transition is not induced by the fission instability [23]. Also, the behavior of χ should be noted; as can be seen from Fig. 4(a), it becomes negative between the phase with rodlike nuclei ($\chi \approx 0$ and $\int_{\partial R} H dA > 0$) and the phase with slablike nuclei ($\chi \approx 0$

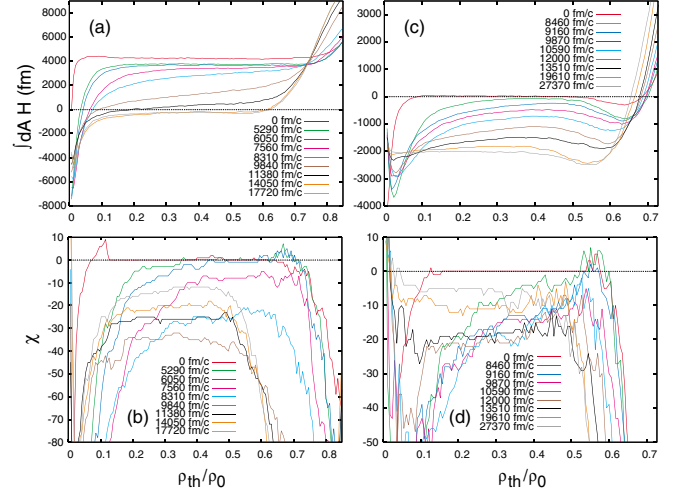


FIG. 3 (color). The quantities $\int_{\partial R} H dA$ and χ as functions of the threshold density ρ_{th} calculated for the nucleon density fields of Fig. 1 [(a) and (b)] and of Fig. 2 [(c) and (d)].

and $\int_{\partial R} H dA \approx 0$). This implies that the transition proceeds through a transient state with “spongelike” structure. The state which gives the smallest χ at $t \approx 9840$ fm/c corresponds to the moment when all of the rodlike nuclei are connected to others by small bridges; after that, the connected nuclear rods relax into slablike nuclei; i.e., the bridges in the slablike structures merge to form the nuclear slabs, and those across the slabs disappear. The whole transition process can be divided into the “connecting stage” and the “relaxation stage” before and after this moment; the former starts when the nuclei begin to touch and it takes ≈ 3000 – 4000 fm/c, and the latter takes more than 8000 fm/c.

The same quantities are shown for the transition from the phase with slablike nuclei to the phase with cylindrical bubbles in Figs. 3(c), 3(d), and 4(b). The initial

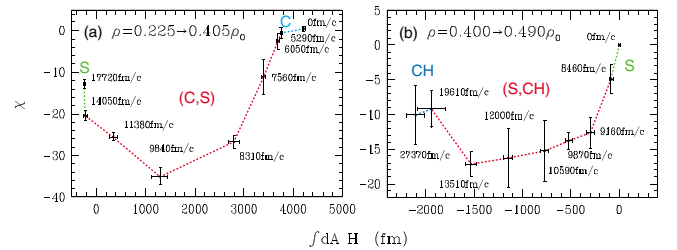


FIG. 4 (color). Time evolution of $\int_{\partial R} H dA$ and χ during the simulations. The data points and the error bars show, respectively, the mean values and the standard deviations in the range of $\rho_{\text{th}} = 0.3$ – $0.5\rho_0$, which includes the values corresponding to the nuclear surface assumed in [20]. We set the averaging range relatively wide because the nuclear surface cannot always be characterized by a single value of ρ_{th} as mentioned in [20]. Panel (a) is for the transition from cylindrical (C) to slablike nuclei (S) and panel (b) for the transition from slablike nuclei to cylindrical holes (CH). Transient states are shown as (C,S) and (S,CH) for each transition.

and the final structures are characterized by the plateau values of $\int_{\partial R} HdA \approx 0$ and ≈ -2000 fm, respectively. From Figs. 3(d) and 4(b), we see that the slablike nuclei begin to touch at $t \lesssim 8460$ fm/c, and the connection of the slablike nuclei by the small bridges are completed at $t \lesssim 12\,000$ fm/c corresponding to the state with the lowest χ . In this case, the connecting stage lasts for ≈ 3000 – 4000 fm/c and the relaxation stage for more than $15\,000$ fm/c. In the latter period, the bridges merge to form cylindrical holes shown by the increase of χ toward zero, and, simultaneously, their positions relax into a triangular lattice as mentioned before.

In conclusion, we have succeeded in simulating the dynamical process of two types of transitions between pasta phases at subnuclear densities. Our calculations support the idea that transitions between pasta phases can occur during stellar collapse. The particular transitions we have examined are triggered by the thermal fluctuation, not by the fission instability. They consist of the connecting stage and the relaxation stage. The total time of the connecting stage is 3000 – 4000 fm/c in our simulations, which could be shortened by the artificial compression. However, we can conclude that the connecting stage would be complete in a time scale of order 10^3 fm/c, taking account of the facts that each connecting process observed in this stage proceeds much faster than the compression and that the time scale of ordinary nuclear fission is about 1000 fm/c. The relaxation stage takes about $10\,000$ fm/c or more. A remaining challenge is to investigate the transition from the bcc lattice of spherical nuclei to the triangular lattice of rodlike nuclei [12]. If this process is confirmed, the existence of the pasta phases in supernova cores will be almost established.

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 [19] According to the typical value of the density difference between each pasta phase, $\sim 0.1\rho_0$, we increase the density to the value corresponding to the next pasta phase taking the order of 10^4 fm/c, which is much longer than the typical time scale of the nuclear fission, ~ 1000 fm/c. Therefore, if a dynamical phenomenon of nuclei whose time scale is less than the order of 10^4 fm/c is observed during the compression, its dynamics is determined by the intrinsic physical properties of the system, not by the density change applied externally, whose time scale is much shorter than that of the actual stellar collapse.
 [20] We here assume that the nuclear surface corresponds to the isodensity surface for a threshold density (see later) of $\rho_{\text{th}} = 0.45$ – $0.5\rho_0$. We should mention that the nuclear surface cannot be characterized by a single value of ρ_{th} except for the state before the fusion and after the system is fully relaxed because the density in the nuclear matter region in the transient states is quite inhomogeneous.
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 [22] The value of χ is positive for the phases with spherical nuclei and spherical bubbles, and is zero for the other ideal pasta phases, i.e., the phases of rodlike nuclei, slablike nuclei, and cylindrical bubbles.
 [23] $\int_{\partial R} HdA$ should decrease before χ deviates from zero if the transition is triggered by the fission instability; i.e., nuclei deform largely before they touch. We see, however, only a minor change of $\int_{\partial R} HdA$ before χ decreases.