Polycrystalline Crusts in Accreting Neutron Stars

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Abstract

The crust of accreting neutron stars plays a central role in many different observational phenomena. In these stars, heavy elements produced by H-He burning in the rapid proton capture (rp-) process continually freeze to form new crust. In this paper, we explore the expected composition of the solid phase. We first demonstrate using molecular dynamics that two distinct types of chemical separations occur, depending on the composition of the rp-process ashes. We then calculate phase diagrams for three-component mixtures and use them to determine the allowed crust compositions. We show that, for the large range of atomic numbers produced in the rp-process ($Z \sim 10$–50), the solid that forms has only a small number of available compositions. We conclude that accreting neutron star crusts should be polycrystalline, with domains of distinct composition. Our results motivate further work on the size of the compositional domains and have implications for crust physics and accreting neutron star phenomenology.

Key words: accretion, accretion disks – dense matter – stars: interiors – stars: neutron – X-rays: binaries – X-rays: bursts

1. Introduction

The structure and composition of accreting neutron star crusts plays a key role in a diverse set of astrophysical phenomena. As the crust is compressed by accretion, nuclear reactions such as electron captures or p-nuclear fusion change the composition and deposit heat (Haensel & Zdunik 2003). In transiently accreting neutron stars, cooling of the hot crust during periods of quiescence has been used to infer properties such as the crust thermal conductivity (Shitermin et al. 2007; Brown & Cumming 2009) and to limit the heat capacity and neutrino emissivity of the neutron star core (Heinke et al. 2010; Cumming et al. 2017; Brown et al. 2018). The electrical conductivity sets the rate of decay of crust currents (Urpin & Geppert 1995; Brown & Bildsten 1998), which is important because accreting neutron stars, as progenitors of millisecond radio pulsars, are believed to be undergoing accretion-driven magnetic field decay (e.g., Konar 2017). Depending on the shear modulus (Horowitz et al. 2007), asymmetries in electron capture layers may give quadrupole moments large enough to limit the spin-up of the neutron star by angular momentum loss from gravitational radiation (Bildsten 1998), potentially observable with next generation gravitational wave observatories (Watts et al. 2008).

Because many accreting neutron stars have accreted enough matter ($\gtrsim 10^{-5} M_*$) to replace their entire crust, it is crucial to understand how freshly accreted matter freezes to form new solids. Freezing is well-understood for a one-component plasma (OCP), which freezes into a bcc lattice when the density is high enough for the Coulomb interactions between nuclei to overcome their thermal motion (e.g., Brush et al. 1966; Potekhin & Chabrier 2000). The material freezing to make the new crust in accreting neutron stars, however, consists of a complex mixture of elements produced by nuclear burning of the accreted H and He via the rp-process (Schatz et al. 1999). Investigations of the lattice structure and freezing point of such mixtures have only started to be carried out more recently (Horowitz et al. 2007, 2009; Horowitz & Berry 2009; Mckinven et al. 2016).

An important process in multicomponent plasmas is chemical separation on freezing. In a molecular dynamics study of one realistic composition, Horowitz et al. (2007) found that light nuclei (low atomic number $Z$) were retained in the liquid phase, with heavier nuclei (high $Z$) going into the solid. This change in composition raises the question of how freezing accommodates the large variety of different abundance patterns that are produced by the rp-process (Schatz et al. 2003). Recently, Mckinven et al. (2016) used a double-tangent-construction method based on analytic fits to free energies to calculate the liquid–solid equilibrium for a large sample of rp-process ashes. They identified a new type of chemical separation for light mixtures in which the solid forms primarily from the most abundant element, with other elements (light and heavy) going into the liquid phase. This opens a channel for a light composition crust to be formed.

In this work, we explore the expected composition of accreting neutron star crusts. We first use molecular dynamics simulations to confirm that two possible phase separations—light and heavy—can occur (Section 2). We then survey the possible solids that can form, using a three-component approximation that allows a calculation of the full phase diagram. We show that, as a consequence of the large range of atomic number $Z$ in the mixture, only a small number of solid compositions are available to form new crust. For a given rp-process ash, the crust must therefore consist of distinct solid phases; accreting neutron stars have a polycrystalline crust whose domains have distinct compositions. In Section 4, we summarize our results and discuss the implications for accreting neutron stars.

2. Molecular Dynamics Simulations of the Phase Separation of a Light Mixture

In this section, we perform a large molecular dynamics simulation to determine the chemical separation on freezing for
one of the light mixtures considered by Mckinven et al. (2016). Their work was based on analytic expressions for the free energy of multicomponent plasmas extrapolated from simulations of two- and three-component plasmas (Ogata et al. 1993; Medin & Cumming 2010); here, we compare their results with a direct molecular dynamics simulation.

Our molecular dynamics simulations treat nuclei as classical point particles with charge $Z_i$ interacting via a two-body potential,

$$V(r_{ij}) = \frac{Z_i Z_j e^2}{r_{ij}} \exp(-r_{ij}/\lambda),$$  \hspace{1cm} (1)

where $r_{ij}$ is the separation between two nuclei. The exponential screening, due to the degenerate electron gas between ions, is

$$\lambda^{-1} = 2\alpha^{1/2} k_F/\pi^{1/2},$$

where the electron Fermi momentum $k_F = (3\pi^2 n_e)^{2/3}$ and $\alpha$ is the fine structure constant. The electron density $n_e$ is equal to the ion charge density, $n_i = (Z/n)$, where $n$ is the ion density and $(Z)$ is the average charge. The screening length is generally greater than the inter-ion spacing due to the high electron Fermi energy in the neutron star crust. We solve Newton’s equations of motion numerically to study the evolution of the material using the Indiana University Molecular Dynamics (IUMD) CUDA-Fortran code, version 6.3.1, which has previously been used to study neutron star crusts (Caplan & Horowitz 2017).

The composition we consider is taken from Schatz et al. (1999); accretion rate $\dot{m} = 0.1 \dot{m}_{Edd}$, helium fraction $Y = 0.2752$, removing species less abundant than $10^{-3}$, and assuming that nuclei with $Z \leq 6$ have burned to Mg ($Z = 12$; the abundances are shown in the right panel of Figure 2). In reality, the burning produces many more different species than are shown here. For simplicity, we include only the 11 most abundant elements. We take all isotopes of the same element to have the mass of the most abundant isotope.

Following the procedure of Horowitz et al. (2007), we first initialize a smaller simulation of 3456 nuclei ($12 \times 12 \times 12$ bcc unit cells) with periodic boundary conditions and use trial and error to find the melting/freezing temperature. We set the density to $n = 7.18 \times 10^{15}$ fm$^{-3}$ (screening length $\lambda = 35.8516$ fm), initial temperature $T_0 = 0.40$ MeV, and timestep $dt = 25$ fm c$^{-1}$. (Although these densities and temperatures are higher than typical conditions at the freezing depth in a neutron star crust, the evolution depends on $T$ and $\rho$ only through the Coulomb parameter $G = (Z^5/3)e^2 / a_{\text{kg}} T$ with $a_e = (3/4 \pi n_e)^{1/3}$, which is chosen here to be near the freezing point). The nuclei were initialized with random positions and with velocities generated from a Maxwell–Boltzmann distribution at the desired temperature with zero net momentum. A trial-and-error process was used to find the freezing temperature over $2240 \times 10^6$ fm c$^{-1}$ (89.6 $\times$ $10^6$ timesteps); first, the simulation was slowly heated to 0.130 MeV by periodically rescaling the velocities and then supercooled to 0.036 MeV where the mixture froze (molecular dynamics simulations tend to freeze nearer 0.9 $T_{\text{melt}}$ due to finite time effects). Coincidentally, when the mixture froze, the crystal planes that formed were parallel with the simulation boundaries (seen in Figure 1). This may be a consequence of simulating with $12^3 \times 2$ nuclei that are able to perfectly fill a cubic simulation volume with a bcc lattice. The crystal was then tiled to make a $2 \times 2 \times 2$ larger volume configuration with 27648 nuclei and then evolved for an additional $400 \times 10^6$ fm c$^{-1}$ ($16 \times 10^6$ timesteps) and heated to $T = 0.042$ MeV, which was believed to be nearer the true melting point. This verified that the larger tiled crystal simulation was stable and would not spontaneously melt at the higher temperature.

A liquid configuration with 27648 nuclei and an identical composition was assembled in a similar way, by tiling a smaller liquid configuration containing 3456 nuclei at $T = 0.0413$ MeV, then equilibrated for $50 \times 10^6$ fm c$^{-1}$ ($2 \times 10^6$ timesteps) at $T = 0.042$ MeV.

The liquid and solid configurations were joined on one face to prepare a configuration with 55296 nuclei, shown in the left panel of Figure 1, the starting point of our simulation of phase separation. This half-solid/half-liquid configuration was evolved for $1200 \times 10^6$ fm c$^{-1}$ ($48 \times 10^6$ timesteps). The initial temperature was 0.042 MeV and was adjusted periodically in order to ensure that half of the simulation volume remained solid while half remained liquid, because the melting temperature is not known precisely in advance (as in Horowitz et al. 2007). These temperature adjustments do not correspond to a physical process in the neutron star; rather, we seek to find the conditions for equilibrium solid–liquid coexistence, which is exactly the condition met by the ocean-crust interface in the neutron star. To verify that the simulation had equal parts solid and liquid, we partitioned the simulation volume into 30 equal sized “slices” along the long axis every $10^7$ fm c$^{-1}$ and determined which slices were solid, liquid, or interfacial by inspection.

The thermodynamic history is shown in the right panel of Figure 1. The simulation equilibrated after $900 \times 10^6$ fm c$^{-1}$ ($36 \times 10^6$ timesteps) at a temperature of 0.044 MeV, with no further changes in abundances or solid and liquid volume fractions. For each nuclear species, we show the ratio $x_i/x_j$ where $x_i(x_j)$ is the number fraction of nuclei of that species found in the solid (liquid) slices. Initially, the solid and the liquid have identical compositions ($x_i/x_j = 1$) for all species. Within $100 \times 10^6$ fm c$^{-1}$ ($4 \times 10^6$ timesteps), the compositions have begun to differentiate, nuclei with $Z = 10–12$ enhanced ($x_i/x_j > 1$) and other species depleted ($x_i/x_j < 1$) in the solid.

We then extracted the final abundance ratios. Accurate identification of which particles in the simulation were in a solid configuration or in a liquid configuration was complicated by the appearance of a liquid subvolume within the crystal (this can be seen in Figure 1). To separate the liquid and solid abundances, we used the local bond order parameter, which quantifies the regularity of bond angles between nearest neighbors. This allows us quantify whether individual nuclei are in a lattice or an amorphous region more reliably than using inspection of domains. We use the method of Wang et al. (2005; following Steinhardt et al. 1983) to calculate the bond order parameter,

$$Q_6 = \sqrt{\frac{4\pi}{2l+1} \sum_{m=-l}^{l} \frac{1}{N_b} \sum_{\text{bonds}} Y_{lm}(\theta(r), \phi(r))}, \hspace{1cm} (2)$$

for each nucleus. The spherical harmonics $Y_{lm}$ are calculated using the angles between pairs of nuclei $\theta(r)$ and $\phi(r)$, averaged over nearest neighbors separated by vector $r$ (number $N_b$ within $|r| < 35$ fm). Nuclei are counted as solid if $Q_6 > 0.4$ and considered liquid if $Q_6 < 0.3$ ($Q_6 = 0.5$ for a zero-temperature
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Molecular dynamics simulation. Left panel: initial and final configurations, with each point representing one nucleus. The simulation is three-dimensional, but an orthographic projection is used here for clarity and shows the bcc (100) surface in the solid. The clustering in the solid is due to the distribution of nuclei in the third dimension; the simulation is approximately a bcc lattice and each point is near a lattice site. The colors are dimmed according to depth in the field and also identify ion species: in order of abundance, they are $Z = 12$ white, $Z = 10$ cyan, $Z = 8$ red, $Z = 18$ blue, $Z = 11$ tan, and the remaining six species (totaling 5% of all ions) shown in yellow. During the simulation, the liquid region has moved over the periodic boundary, and a subregion of liquid has developed within the solid region (see text for discussion). Right panel: thermodynamic history showing the evolution of abundances in the solid and liquid, thermal history (with energy per nucleus $e$), and volume fractions.

These cut-offs exclude approximately one-third of our points, which are mostly near the interfaces or in the mixed region.

Figure 2 shows the final abundance ratios compared with the results from Mckinven et al. (2016). The agreement is excellent, with the solid enhanced in $Z = 10–12$ nuclei and depleted in heavier nuclei. This confirms the finding of Mckinven et al. (2016) that light mixtures phase separate differently than heavy mixtures. For comparison, we show in the left panel the molecular dynamics results of Horowitz et al. (2007) for a heavy mixture. Heavy mixtures freeze a solid made up primarily of large $Z$ nuclei, with light elements staying in the liquid phase. Light mixtures on the other hand form a solid from the most abundant element. Depending on the composition, the solid can be lighter or heavier than the starting composition.

### 3. Three-component Phase Separation

Next, we calculate the phase diagram for a three-component mixture that approximates rp-process ashes, using it to explore the solid compositions that form. To model light, medium, and heavy elements, we consider a three-component mixture with $Z_1 = 9$, $Z_2 = 12$, and $Z_3 = 22$, with fractional abundances of each species $x_i$ (defining composition $\mathbf{X} = (x_1, x_2, x_3)$). We use the double-tangent construction (e.g., Gordon 1968) to identify unstable regions of the phase diagram, as described by Medin & Cumming (2010). To compute the free energies of liquid and solid phases, we follow Medin & Cumming (2010), specifically their Equation (9) for the difference between the liquid and solid free energies for a OCP (based on Dubin 1990 and Dewitt & Slattery 2003), and their Equations (23) to (25) for the multicomponent liquid and solid (based on Ogata et al. 1993).

To briefly summarize our method, we begin with the free energies for solid and liquid mixtures,

$$f_i^{\text{MCP}}(\Gamma_i, x_1, \frac{x_2}{Z_2}, \frac{x_3}{Z_3}) \simeq \sum_{i=1}^{3} x_i \left[ f_i^{\text{OCP}}(\Gamma_i) + \ln \left( \frac{x_i}{Z_i} \right) \right]$$

(3)

and

$$f_x^{\text{MCP}}(\Gamma_1, x_1, \frac{x_2}{Z_2}, \frac{x_3}{Z_3}) \simeq \sum_{i=1}^{3} x_i \left[ f_x^{\text{OCP}}(\Gamma_i) + \ln \left( \frac{x_i}{Z_i} \right) \right] + \delta f_x(\Gamma_1, x_1, \frac{x_2}{Z_2}, \frac{x_3}{Z_3})$$

(4)

with free energies for the one-component solid $f_i^{\text{OCP}}$ and liquid $f_x^{\text{OCP}}$, and a deviation from linear mixing for the solid $\delta f_x$ (from Medin & Cumming 2010). Each species is characterized by its one-component Coulomb parameter, $\Gamma_i = Z_i^{5/3} e^2/\alpha_i k_B T$, as defined in the previous section. We use $\Gamma_1$ as a proxy for temperature, where increasing $\Gamma_1$ corresponds to increasing temperature ($\Gamma_2$ and $\Gamma_3$ can be found straightforwardly from $\Gamma_1 \equiv (Z_i/Z_1)^{5/3} \Gamma_i$). The one-component melting temperature for component one is $\Gamma_1 = \Gamma_c = 178.6$; the one-component melting temperature for component two is $\Gamma_1 = (Z_1/Z_2)^{5/3} \Gamma_c = 110.6$; and the one-component melting temperature for component three is $\Gamma_1 = (Z_1/Z_3)^{5/3} \Gamma_c = 40.3$.
We use these free energies to find compositions that are unstable to phase separation. To do this, we identify pairs of points on the minimum free energy surface which share a tangent plane (i.e., the double-tangent construction). Pairs of points found via the double-tangent construction (i.e., pairs $X_s$ and $X_l$) correspond to solid compositions and liquid compositions that can coexist (i.e., phase separation). In Figure 3, we plot all liquid compositions $X_l$ found via the tangent construction in orange, with their corresponding solid composition $X_s$ in blue. Connecting them in green are tie lines, which span a metastable space. Any composition along this line will spontaneously separate into a solid with composition $X_s$ and a liquid with composition $X_l$. Thus, the region bounded by the orange curve consists of all stable liquid compositions, the region bounded by the blue points (for example along the $x_2$ axis and in the bottom left corner) consists of stable solid, while the remaining space in the phase diagram denotes an unstable region. In the unstable region, the mixture can lower its free energy by phase separating into a solid and liquid of the solidus and liquidus compositions at each end of the tie lines. For clarity, we show only tie lines connecting liquidus and solidus points; tie lines for solid–solid equilibria are not shown.

The results are shown in Figure 3 for four different values of $\Gamma_1$. For the free energy fits used here, an OCP of species 1 would melt when $\Gamma_1 = \Gamma_c = 178.6$. However, a small amount of the heavy species 3 added to the mixture lowers the melting point, causing a liquid region to appear even for $\Gamma_1 > \Gamma_c$ (top left of Figure 3). As $\Gamma_1$ decreases, the liquidus sweeps across the phase diagram as progressively more mixtures are able to melt.

The striking feature of Figure 3 is that the solidus points are confined to the boundaries. Solids that form are either composed almost entirely of the heaviest element or are a mixture of species 1 and 2 and completely depleted in the heaviest element. This matches the behavior of the multi-component mixtures in Figure 2 and is a result of the large charge ratio of the rp-process ashes. Ogata et al. (1993) showed for two-component plasmas that increasing the charge ratio between components significantly increases the free energy of the solid (see Figure 3 of Ogata et al. 1993). This leads to an increasing preference for the mixture to phase separate into almost pure solids. As the charge ratio increases, the two-component phase diagrams progress from azeotropic/spindle type, with only a small difference between liquid and solid compositions, to eutectic type, with a large difference between liquid and solid (see Figure 5 of Ogata et al. 1993 and Section 2.1 of Medin & Cumming 2011). We see a similar effect here for three-components. Previous studies of three-component plasmas focused on C–O–Ne mixtures for white dwarfs and found only small phase separations (Ogata et al. 1993; Segretain & Chabrier 1993; Hughto et al. 2012).
4. Implications for Accreted Crusts

Both molecular dynamics with a full rp-process ash composition and a three-component approximation show that newly forming crust in accreting neutron stars has a limited number of compositions available. This means that for any given incoming mixture produced by the rp-process, there is not likely to be a solid with that composition that can form in equilibrium with the liquid at the base of the neutron star ocean. However, if multiple domains of distinct composition can form, then on average, the ocean can reach a steady state and deposit out the incoming mixture. Figure 3 suggests a mechanism by which this could happen, as it shows that small changes in the liquid composition lead to dramatically different solid compositions. This can in fact be seen in the multicomponent results of Mckinven et al. (2016). Figure 4 shows two compositions from that paper that are very similar yet phase separate differently (one in the same way as the light mixture and the other in the same way as the heavy mixture in Figure 2). The red point in the upper right panel of Figure 3 shows roughly where this mixture would lie in our three-component approximation. Small changes in the ocean composition (point $L = (x_1 = 0.46, x_2 = 0.46, x_3 = 0.08)$) would cause the solid to alternate between two compositions, one light (point $A = (x_1 = 0.32, x_2 = 0.68, x_3 = 0.00)$) and one heavy (point $B = (x_1 = 0.01, x_2 = 0.01, x_3 = 0.98)$). The solid–liquid ratios between A–L and B–L are indicated in Figure 4 and agree well with the multicomponent results.

The idea of a polycrystalline crust composed of microscopic domains has been discussed before for a single composition (e.g., Kobyakov & Pethick 2015). Here, we see that formation of domains with different compositions is a natural outcome of the freezing of a many-component plasma. Support for this picture comes from molecular dynamics simulations of the solid phase (Horowitz et al. 2009), in which a solid initially created with one specific rp-process ash mixture phase separated into two solid components. In addition, when the composition was depleted in light elements, a single stable solid formed, with light nuclei occupying interstitial sites in the crystal lattice (Horowitz & Berry 2009). Although our
three-component approximation suggests that two solid phases form, in general many-component mixtures with large charge ratios may seek to form more than two crystal compositions. Our calculation does not specify the size of the compositional domains. They may take the form of microscopic grains with characteristic sizes determined by diffusion lengths if steady state deposition occurs. In that case, the ocean adopts a specific mixture (such as point L in Figure 3) and simultaneously freezes out multiple solids. Diffusion could cause the domains to merge in the outer crust (Mckinven et al. 2016), although the diffusion rate drops exponentially and the tendency for separation into pure solid components increases at higher $\Gamma$ (Ogata et al. 1993). Alternatively, the crust composition could switch on an astrophysical timescale associated with changing ocean composition, as rp-process burning conditions change and as the ocean composition adjusts in response to losses to the crust. In that case, the domain size could be a significant fraction of the scale height ($\sim 10$ m). Further work is needed to model compositional transport through the ocean, which will also have implications for X-ray bursts and superbursts. The fact that a three-component approximation is able to reproduce the phase separation of multicomponent mixtures suggests it may be promising to include in time-dependent simulations.

Several aspects of crustal physics should be revisited considering compositional domains. For example, new investigations into the transport properties of a polycrystalline crust are needed. While phase separation acts to increase the purity of the solid (so that individual domains should have a higher conductivity than the average composition), grain boundaries between microscopic grains may enhance electron scattering. Characterizing the crust with a single impurity parameter (e.g., Itoh & Kohyama 1993) may not be sufficient. The behavior of compositional domains as they undergo electron captures and other crust reactions will be important to study. In particular, the evolution of compositional domains through the crust may influence the size of the mass quadrupole associated with electron capture layers, a possible source of gravitational waves. Likewise, the partitioning of different species into domains may change pycnonuclear reaction rates (Yakovlev et al. 2006; Horowitz et al. 2008), a source of crustal heating. In addition, a growing body of recent work is similarly emphasizing and investigating the importance of the transport and elastic properties of anisotropic materials in the crust (such as in crystalline domains and nuclear pasta; Kobyakov 2017; Duriel & Urban 2018; Kobyakov & Pethick 2018).

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