Binary and ternary ionic compounds in the outer crust of accreted neutron stars

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Binary and ternary ionic compounds in the outer crust of accreted neutron stars

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Abstract. The outer crust of an accreted neutron star is thought to contain a large distribution of different nuclear species resulting from the burying of ashes of X-ray bursts and superbursts. By analysing the stability of multicomponent Coulomb crystals against phase separation, it is found that various binary and ternary ionic compounds could be formed.

1. Introduction

Many properties of the crust of a neutron star depend to a large extent on its structure, which in turn have implications for various astrophysical phenomena, such as Crab like pulsar sudden spin-ups, thermal relaxation in transiently accreting stars, giant flares from soft gamma-ray repeaters, and gravitational-wave emission (see, e.g., Ref. [1]).

The outermost region of a neutron star is expected to be made of iron $^{56}$Fe, the end-product of stellar nucleosynthesis. The properties of compressed iron can be probed in terrestrial laboratories up to pressures of order $10^{14}$ dyn cm$^{-2}$ (densities of a few tens of g cm$^{-3}$) with nuclear explosions and laser-driven shock-wave experiments. Under these conditions, iron has an hexagonal close-packed structure [2]. Ab initio calculations predict various structural phase transitions at higher pressures. Although such pressures are tremendous according to terrestrial standards, they still remain negligibly small compared with those prevailing in a neutron star. Deeper in the star, at a density $\rho_{\text{eip}} \approx 2 \times 10^{4}$ g cm$^{-3}$, the interatomic spacing becomes comparable with the atomic radius. At densities $\rho \gg \rho_{\text{eip}}$, atoms are crushed into a dense Coulomb plasma of atomic nuclei in a charge compensating background of highly degenerate electrons. The denser regions of the crust are expected to be stratified into a succession of layers with different compositions. The onset of neutron emission at densities $\rho_{\text{drip}} \sim 10^{11}$ g cm$^{-3}$ delimits the boundary between the outer and inner regions of the crust (see, e.g., Ref. [3]).

It has long been assumed that each layer of the outer crust consists of a body-centered cubic (bcc) crystal made of a single nuclear species [4]. The stratification of the crust (see, e.g. Refs. [5, 6, 7, 8]) is mainly a consequence of the cold catalysed matter hypothesis [9, 10]. Because neutron stars are formed from gravitational core-collapse supernova explosions with temperatures exceeding $10^{10}$ K, their interior is thought to be in full thermodynamic equilibrium. As the star cools down by emitting neutrinos, the distribution of nuclides shrinks, and eventually reduces to one or two species at absolute zero temperature (see, e.g. Ref. [11]). However, nuclear processes in the outer envelope of the star are likely to be quenched after the crystallisation (see, e.g., Ref. [1] and references therein). Moreover, the constitution of neutron-star crusts may differ...
from that of cold catalysed matter due to the fallback of material from the envelope ejected during the supernova explosion and due to the accretion of matter from a stellar companion.

In the presence of different nuclear species, various solid structures may form. We have recently studied the formation of multinary compounds in dense stellar matter, and analysed their stability [8]. We have found that substitutional binary compounds with cesium chloride structure are generally present at the interface between adjacent layers in the outer crust of a cold nonaccreted neutron star [8], as first shown in Ref. [12]. In this paper, we pursue our investigations in accreted neutron-star crusts.

2. Formation of multinary ionic compounds in accreted neutron-star crusts

The accretion of matter from a stellar companion onto a neutron star forms an hydrogen-rich envelope. Stable hydrogen burning produces helium, and depending on the accretion rate, unstable helium burning converts within seconds all the envelope into nuclides in the nickel-cadmium range, leading to X-ray bursts. Less frequent but more energetic are superbursts presumably triggered by unstable carbon burning. Ashes of these thermonuclear explosions may be further processed as they sink deeper inside the star (see, e.g., Ref. [1]).

The equilibrium structure of such multicomponent plasmas remains highly uncertain. According to classical molecular dynamics cooling simulations of hot plasmas, nuclei tend to crystallize into a bcc lattice, as in nonaccreted crusts [13]. However, the system may have not fully relaxed to its true equilibrium state due to the very slow dynamics of crystal growth. Moreover, these simulations were performed at fixed ion number densities, and may not represent the conditions prevailing in neutron stars since the density does not necessarily vary continuously throughout the stellar interior contrary to the pressure. Recently, a different approach has been followed to find the ground-state configuration (at zero temperature and fixed pressure) using genetic algorithms [14]. But such unconstrained global searches of the equilibrium structure remains computationally costly, and for this reason have been restricted to the ternary systems O-Fe-Se, and Fe-As-Se considering polycrystalline mixtures of stoechiometric compounds at two different values of the pressure.

A thermodynamically favorable condition for a multinary compound made of nuclei with charges \{Z_i\} to exist in the crust of a neutron star is the stability against the separation into pure (bcc) phases [8] (unstable compounds might still exist depending on how fast ions diffuse). Indeed, coexisting phases separate and settle to different depths due to gravity. As shown in Ref. [8], the stability condition of any compound at zero temperature is independent of the stellar environment (neglecting electron exchange and correlation, electron charge polarisation, and quantum-zero point motion of ions about their equilibrium positions), and is embedded in the following inequality:

\[
R(\{Z_i\}) \equiv \frac{C}{C_{\text{bcc}}} f(\{Z_i\}) \frac{Z}{Z^{2/3}} > 1,
\]

where \(R\) is the ratio of the electrostatic energy of the compound to that of coexisting bcc phases, \(f(\{Z_i\})\) is the dimensionless structure function of the compound, \(C\) the corresponding structure constant\(^1\), \(C_{\text{bcc}} = -1.444231\) the structure constant of a bcc lattice [15], and overlined symbols indicate mean values (e.g. \(\bar{Z} \equiv \sum_i Z_i\xi_i\), where \(\xi_i\) denotes the relative abundance of nuclei \(i\)).

For compounds made of isotopes with the same charge \(Z\), the structure function reduces to \(f(Z) = Z^{2/3}\). For multicomponent systems with different charges \{Z_i\}, the quantity \(R\) only depends on the charge ratios \(Z_i/Z_j\) with \(i \neq j\). In particular, the function \(R(Z_1, Z_2, Z_3)\) of a ternary compound can be expressed as \([8]\)

\[
R(q, p) = \frac{C}{C_{\text{bcc}}} \frac{\eta_1 + \eta_2 q^2 + \eta_3 p^2 + \eta_12 q + \eta_13 p + \eta_23 qp}{(\xi_1 + \xi_2 q + \xi_3 p)^{1/3}(\xi_1 + \xi_2 q^{2/3} + \xi_3 p^{2/3})},
\]

\(^1\) The structure constant \(C\) is related to the Madelung constant \(C_M\) by \(C = C_M(4\pi/3)^{1/3}\).
where \( q \equiv Z_2/Z_1 \) and \( p \equiv Z_3/Z_1 \). The (dimensionless) coefficients \( \eta_1, \eta_2, \eta_3, \eta_{12}, \eta_{13}, \) and \( \eta_{23} \) are determined by the spatial arrangement of ions. The function \( R(Z_1, Z_2) \) of a binary compound can be easily inferred from Eq. (2). A compound may be ordered or disordered depending on its composition (see, e.g. Ref. [16]). However, the existence of amorphous solids in accreted neutron-star crusts was found to be incompatible with the observed thermal emission [17]. Therefore, we focus on crystalline compounds.

As shown in Ref. [8], stellar compounds having the same structure as auricupride (AuCu₃), fluorite (CaF₂), and tungsten carbide (WC) are not thermodynamically favored \( (R \leq 1) \). Structures similar to that of rocksalt (NaCl), cesium chloride (CsCl), and cubic perovskite (BaTiO₃), shown in Fig. 1, can lead to thermodynamically favored compounds depending on the composition (including binary compounds based on the cubic perovskite structure with \( Z_1 = Z_3 \) or \( Z_1 = Z_2 \)). We have also considered the binary compound (3) proposed by Dyson [18]. The values for the structure constants are indicated in Table 1. The structure function of Dyson’s compound was calculated as follows [19]: \( \eta_1 = C_{\text{bcc}}/(4^{1/3} C_{\text{sc}}) \), \( \eta_2 = \eta_1 + 1/2 \), \( \eta_{12} = 1 - \eta_1 - \eta_2 \), and \( C_{\text{sc}} = -1.418649 \) is the structure constant of a simple cubic lattice taken from Ref. [12]. Dyson’s compound is found to be thermodynamically favored for small charge ratios \( q < 0.0181571 \), with \( R \) reaching 1.0003 for \( q \approx 0.0076 \). The ratio \( R \) obtained from Eq. (2) for the CsCl structure coincides with the inverse of Eq. (5) given in Ref. [20] with \( q = \alpha \), \( C = (4\pi/3)^{1/3} \zeta_2 \), \( \eta_1 = \eta_2 = \zeta_1/(2^{1/3} \zeta_2) \), and \( \eta_{12} = 1 - 2 \eta_1 \). We have analysed the stability against phase separation of binary and ternary compounds that could potentially exist in the crust of an accreted neutron star using the nuclear abundancies given in Table I of Ref. [13]. Thermodynamically favored compounds are listed below.

- Rocksalt structure: AgNe.
- Cesium chloride structure: AgCa, AgTi, AgCr, AgFe, AgCo, AgNi, AgZn, AgGe, AgAs, AgSe, AgKr, KrCa, KrTi, KrCr, KrFe, KrCo, KrNi, KrZn, KrGe, KrAs, KrSe, SeCa, SeTi, SeCr, SeFe, SeCo, SeNi, SeZn, SeGe, SeAs, AsCa, AsTi, AsCr, AsFe, AsCo, AsNi, AsZn, AsGe, GeCa, GeTi, GeCr, GeFe, GeCo, GeNi, GeZn, ZnCa, ZnTi, ZnCr, ZnFe, ZnCo, ZnNi, NiCa, NiTi, NiCr, NiFe, NiCo, CoCa, CoTi, CoCr, CoFe, FeCa, FeTi, FeCr, CrCa, CrTi, TiCa.
- Perovskite structure: AgNeO₃.

Binary compounds indicated in boldface are consistent with nuclear abundancies: they could accommodate all available nuclei with the corresponding charges \( Z_1 \) and \( Z_2 \). Compounds with CsCl structure appear to be dynamically stable (against lattice vibrations) since \( q \leq 3.6 \) [20, 21]. With \( q = 4.7 \), AgNe might be dynamically unstable. This analysis might suggest that the crust of an accreted neutron star would generally consist of a mixture of various compounds and pure bcc crystals. However, the coexistence of different phases appears unlikely due to gravitational settling, as argued in Ref. [8] (see also Ref. [14]). This warrants further studies.

**Table 1.** Structure constants of the stellar compounds shown in Fig. 1.

|     | \( C \)       | \( \eta_1 \) | \( \eta_2 \) | \( \eta_3 \) | \( \eta_{12} \) | \( \eta_{13} \) | \( \eta_{23} \) |
|-----|---------------|--------------|--------------|--------------|----------------|----------------|--------------|
| NaCl| -1.418649     | 0.403981     | 0.403981     | 0            | 0.192038       | 0              | 0            |
| CsCl| -1.444231     | 0.389821     | 0.389821     | 0            | 0.220358       | 0              | 0            |
| Dyson| -1.418649    | 0.160330     | 0.660330     | 0            | 0.179340       | 0              | 0            |
| BaTiO₃| -1.36588     | 0.121479     | 0.121479     | 0.514083     | 0.0686701      | 0.149645       | 0.0246441    |
3. Conclusions

We have found that contrary to catalysed neutron-star crusts, various compounds could potentially exist in the crust of an accreted neutron star. If confirmed, their presence may have important implications for the thermal and mechanical properties of the crust [20, 21, 22]. However, our analysis has been restricted to a few binary and ternary compounds at zero temperature, and we have ignored the influence of electron exchange, electron polarisation, and quantum zero-point motion of ions. Moreover, the structure of the crust might depend on the cooling history of the star, and on the crystallisation process. This deserves further studies.

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Figure 1. Stellar compounds considered in this work with examples of terrestrial compounds. The structure labelled “Dyson” was proposed by Freeman Dyson in 1971 [18].