Molecular Dynamics of the Neutron Star Crust: Freezing and Chemical Separation

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Outline

Neutron Star Crust

How is a Neutron Star crust formed?

- Neutron Star accretes material from a companion star.
- Accreted material undergoes nuclear reactions.

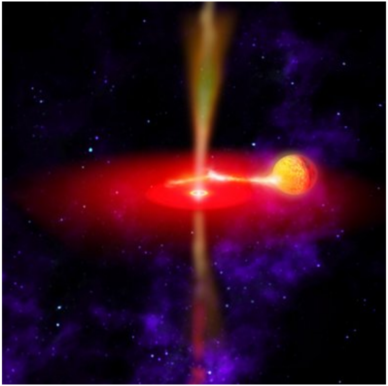


Figure: NASA concept of Cygnus X3.

Neutron Star Crust

What is the composition of the crust?

- Rapid proton capture (rp-process) $\Rightarrow$ medium mass nuclei are synthesized.
- Ash of rp-process is buried by further accretion and density increases.
- Electron capture occurs $\Rightarrow$ nuclei become neutron rich.
- Further accretion pushes mixture deeper into the star and density increases further.
- At $\sim 10^{10}$ g/cm^3 freezing and chemical separation occurs.

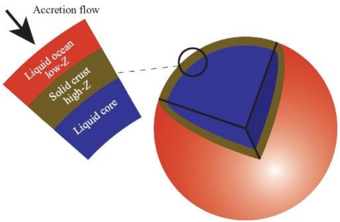


Figure: Schematic diagram of an accreting neutron star.

Multicomponent System

Molecular Dynamics of a 17 component plasma (Horowitz *et al.* 2007).

- Start system with composition expected near the ocean-crust interface of accreting neutron stars (Gupta *et al.* 2007).
- Evolve the system keeping it half solid half liquid;
- Obtain phase transition temperature;
- Observe phase separation.

Multicomponent System

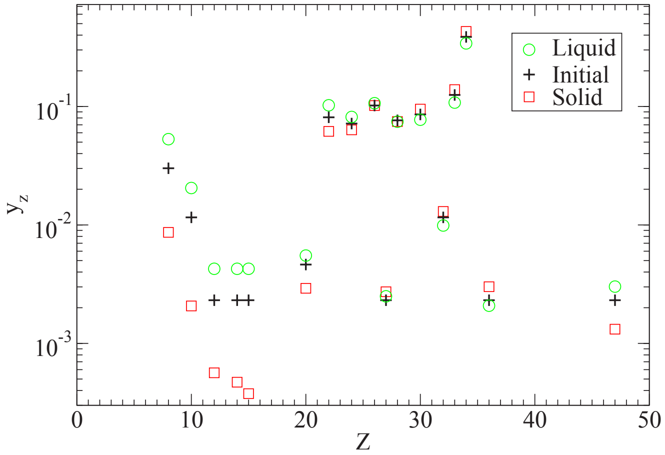


Figure: Number abundance y_Z vs atomic number Z.

Multicomponent System

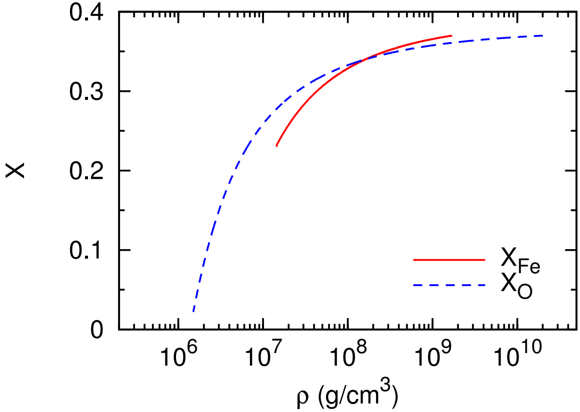


Figure: Composition profile in the convection zone of a $T = 3 \times 10^8$K ocean composed of ^{56}Fe-^{79}Se (solid line) and ^{16}O-^{79}Se (dashed line). Model by Medin and Cumming 2010.

Carbon Oxygen in a White Dwarf Star

Simulation with 55296 ions.

- Set Carbon to Oxygen ratio.
- Make a half-solid half-liquid system.
- Evolve system adjusting the temperature to keep solid to liquid ratio approximately constant.
- Look at properties of the system in both phases.
- Equilibrate the system for a long time:

$$t \simeq 2 \times 10^6 / \bar{\omega}_p$$

where

$$\bar{\omega}_p = \left[\frac{4\pi e^2 \langle Z \rangle^2 n}{\langle M \rangle} \right]^{1/2}$$

is the plasma frequency.

Carbon Oxygen in a White Dwarf Star

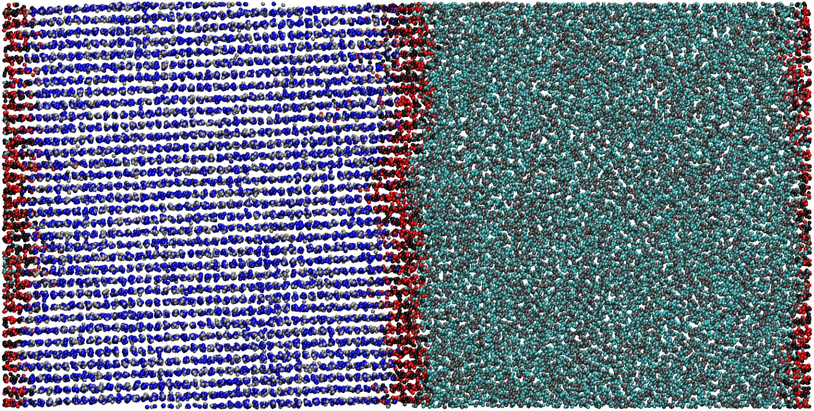


Figure: Final 50%^{12}C and 50%^{16}O configuration. Colors indicate different phases. Silver, Red, Green: ^{12}C in solid, interface and liquid. Blue, Black, Grey: ^{16}O in solid, interface and liquid.

Carbon Oxygen in a White Dwarf Star

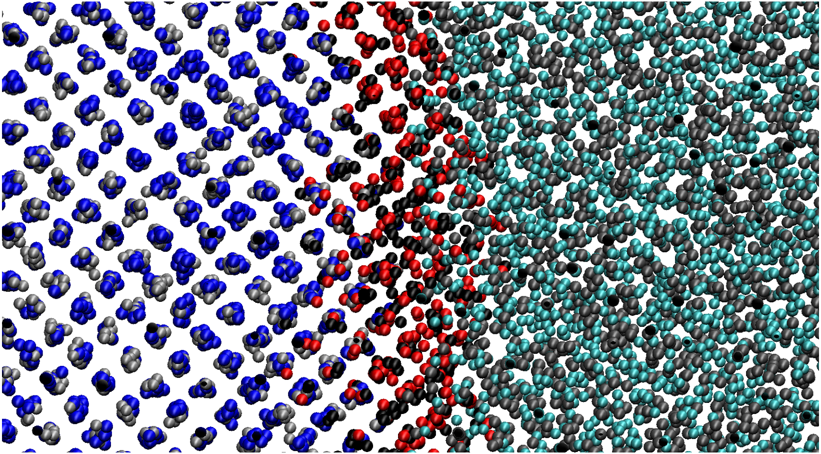


Figure: Close-up on final 50%^{12}C and 50%^{16}O configuration. Colors indicate different phases. Silver, Red, Green: ^{12}C in solid, interface and liquid. Blue, Black, Grey: ^{16}O in solid, interface and liquid.

Phase determination

Define a local orientation order parameter for each ion i

$$\bar{q}_{lm}(i) \equiv \frac{\sum_{j=1}^{N_i} Y_{lm}(\hat{\mathbf{r}}_{ij})\alpha(r_{ij})}{\sum_{j=1}^{N_i} \alpha(r_{ij})}.$$

- $\alpha(r_{ij})$ is a weight function;
- N_i are ions within a (chosen) distance r_{cut} of ion i.

The $\bar{q}_{lm}(i)$ are complex components of a vector in $(2l+1)$ dimensions. Define a dot-product (rotational invariant)

$$\mathbf{q}_l(i) \cdot \mathbf{q}_l(j) = \sum_m \tilde{q}_{lm}(i)\tilde{q}^*_{lm}(j).$$

The $\tilde{q}_{lm}(i)$ are the normalized $\bar{q}_{lm}(i)$, such that $\mathbf{q}_l(i) \cdot \mathbf{q}_l(i) = 1$.

Phase determination

The $l = 6$ order parameter is the most sensitive to our crystalline structure.

- If $\mathbf{q}_l(i) \cdot \mathbf{q}_l(j) \geq 0.5$ particles are connected.
- If $\mathbf{q}_l(i) \cdot \mathbf{q}_l(j) < 0.5$ particles are not connected.

If a particle i is connected to

- more than 80% of its neighbors it is labeled solid;
- less than 20% of its neighbors it is labeled liquid;
- more than 20% and less than 80% it is labeled interface.

Carbon Oxygen

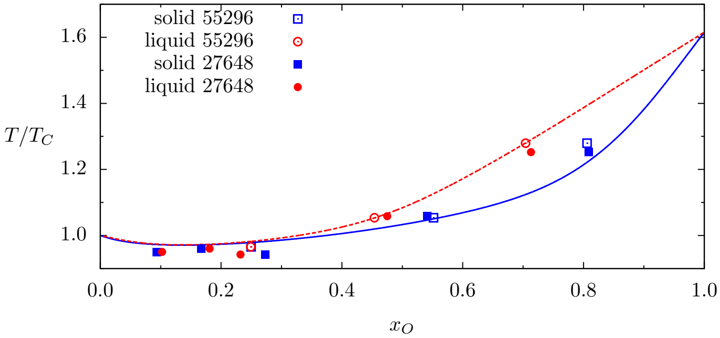


Figure: Phase Diagram for Carbon Oxygen mixture. Curves are from a analytic model by Medin and Cumming 2010.

Carbon Oxygen Neon

- Knowing the phase diagram allows for better determination of stellar age, composition, ...
- Neon ^{22}Ne sedimentation may be an important source of energy during the cooling of a White Dwarf Star.
- Knowing how the Neon phase separates as the star freezes could also be important for Type Ia Supernovae.

Carbon Oxygen Neon

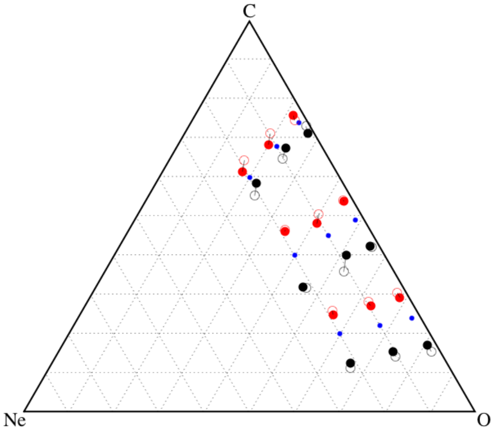


Figure: Phase Diagram for Carbon Oxygen Neon mixtures. Blue dots are the initial composition. Closed black (red) dots is the solid (liquid) composition obtained from the MD simulation. Open black (red) dots is the solid (liquid) composition obtained by Medin and Cumming.

Selenium Oxygen

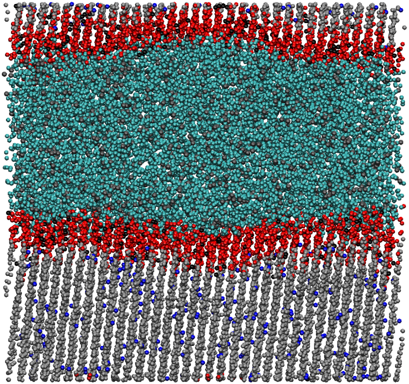


Figure: Selenium 90% Oxygen 10% system. Silver, Red, Green: ^{80}Se in solid, interface and liquid. Blue, Black, Grey: ^{16}O in solid, interface and liquid.

Selenium Oxygen

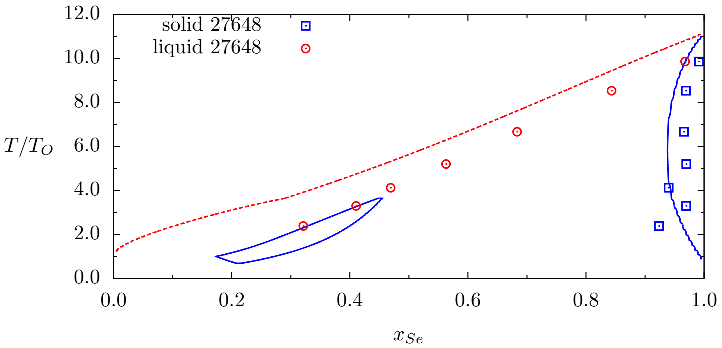


Figure: Phase Diagram for Selenium Oxygen mixture. Curves are from a analytic model by Medin et Cumming.

Selenium Oxygen

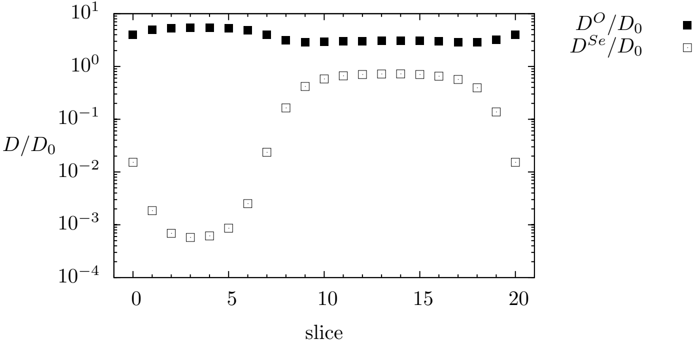
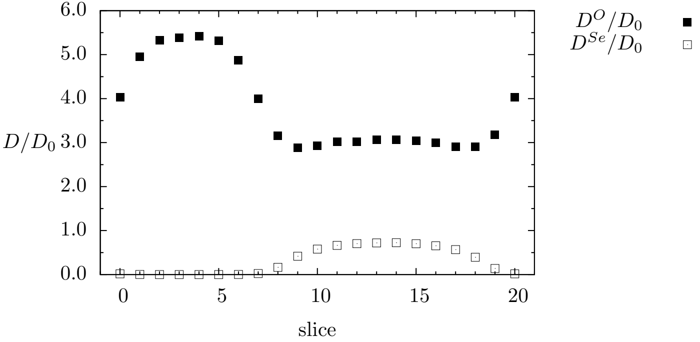


Figure: Diffusion coefficients for selenium and oxygen along the box for the $x_{Se} = 0.90$ system. Slice 1 (20) is the bottom (top) of the box.

Selenium Oxygen



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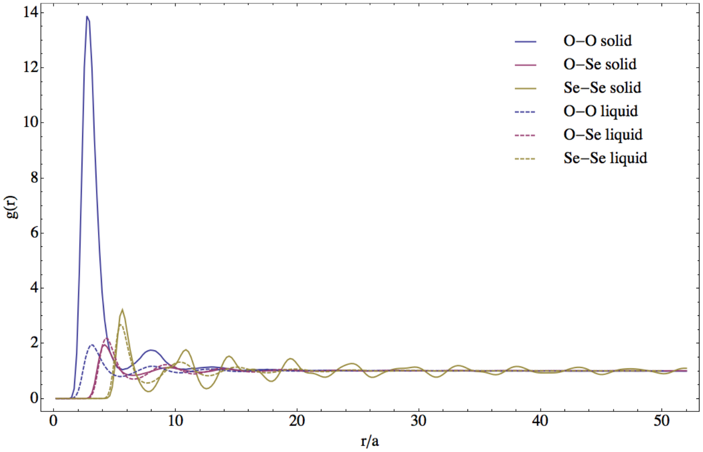

Figure: Correlation functions of elements in the bulk of the solid and liquid.

Conclusions and Future Work

Though computationally expensive MD can

- be used to study phase diagram and dynamical properties of dense plasmas (WD interiors and NS crust);
- give us insights and data which can be used to build analytical models.

Future: Use MD to study more complex phase diagrams.

Suggestions?