Calculating Melting Curves for Crystallizing Stars

From dense plasma physics to stellar archeology

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2020-11-05

Slides: LA-UR-20-28803
1. What are white dwarfs and why are they interesting?

2. Core crystallization

3. Phase diagram calculation

4. Other relevant content
1. What are white dwarfs and why are they interesting?

2. Core crystallization

3. Phase diagram calculation

4. Calculation of...
97% of stars end their lives as white dwarfs
Anatomy of a white dwarf

- **C/O core (99% \( M_{WD} \))**
- **Thick He envelope (10^{-2} M_{WD})**
- **Thin H layer (<10^{-4} M_{WD})**

- Mass: 0.6 \( M_\odot \)
- Density: \( 10^6 \) – \( 10^8 \) g/cm\(^3\)
- Temperature: \( 10^5 \) – \( 10^8 \) K
- Density: 0 – 2 g/cm\(^3\)
- Temperature: 3000 – \( 10^5 \) K
White dwarf cooling

White dwarfs cool down monotonically for their lives.

The age of a white dwarf can be obtained from its:
- temperature
- mass
- atmospheric composition
White dwarf cosmochronology

Using this method, it has been possible to measure the age of the major components of the Milky Way Galaxy.
Stellar archeology

White dwarf cosmochronology is used to infer stellar formation, allowing a detailed reconstruction of the history of our Galaxy.

Such applications demand accurate cooling models.

Likely merger with a satellite galaxy.
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4. Other...
White dwarf core crystallization

WDs undergo a liquid → solid phase transition that needs to be accurately modeled to unlock the power of precision cosmochronology.
Identifying the observational signature of core crystallization

It took 50 years to discover the observational signature of core crystallization.

To distinguish the effect of core crystallization from convective coupling, mass measurements were needed.
How the Gaia satellite provided mass measurements

ESA’s Gaia satellite has increased by a factor of 10 the number of known white dwarfs (now ~250,000)

Launched in 2013, first major data release in 2018

Gaia measures **stellar parallaxes** with an unprecedented accuracy
How the Gaia satellite provided mass measurements

\[
\text{Observed flux} = \frac{\pi R^2}{D^2} \times \text{Surface flux}
\]

Gaia measurements  \quad \text{WDs follow a well-defined mass-radius relationship}

In the pre-Gaia era, there was a degeneracy between \( R \) and \( D \) for most white dwarfs

Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA
The signature of core crystallization

The effect of core crystallization is best seen in the luminosity function of massive WDs
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4. (Blank)
Carbon/oxygen phase separation

H/He envelope

Liquid C/O

O-enriched solid

Solid C/O

Less O

More O

The crystallization from upward as the core contracts.

The new crystals form a solid-liquid interface and are less oxygen compared to the liquid.

 Gradually, a concentration is built, thereby releasing gravitational energy.
The carbon/oxygen phase diagram

1. The liquid cools at constant concentration until it reaches the liquidus line.

2. The liquid coexists with a phase that contains more oxygen.

3. As the crystallization progresses, the liquid becomes impoverished in O.
The carbon/oxygen phase diagram

1. The liquid cools at constant concentration, reaches the liquidus.

2. The liquid coexists with a solid that contains more oxygen.

3. As the crystallization progresses, the liquid becomes impoverished in Oxygen.

4. This process evolves when the azeotropic point is reached.
Previous attempts at computing the C/O phase diagram

**Option 1: Analytical free energy models**

Need to interpolate sparse simulation data, so results are **sensitive to arbitrary choices** made when building the interpolation functions.

Even the *qualitative* shape of the phase diagram is affected by those choices (DeWitt et al. 1996)

\[ f_{\text{mix}} = x_1 f_{\text{OCP}}(\Gamma_1) + x_2 f_{\text{OCP}} \]

fitted to MC calculation

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Hitchcock & Hall 1999
Previous attempts at computing the C/O phase dia

Option 2: Two-phase MD simulations

A solid-liquid interface is simulated and ions are allowed to diffuse

Very costly and sensitive to finite-size effects
The Gibbs-Duhem integration technique

Technique previously developed for neutral mixtures; we have extended it to plasmas.

Relies on the Monte Carlo outputs and the Clapeyron equation:

$$\frac{dP}{dT} = \frac{\Delta S}{\Delta V}$$

Integration along the line of coexistence curve in the fugacity space.
Semigrand canonical MC simulations

1. Ion displacement
   Limited for solid (bcc) phase

2. Volume change

3. Identity change

The volume and the number of ions of each species are not fixed (but $P$ and $N_{tot}$ are).

Those steps insure that the energy is minimized and that the targeted pressure and fugacity fraction ($\xi_0$) are reached.
Semigrand canonical MC simulations

The choice of the type of MC move is randomly chosen at each iteration: particle displacement or volume change or identity change.

The overall acceptance probability of a move is \( \min(1, e^\Lambda) \), where

\[
\Lambda = -\beta(U^{\text{trial}} - U^{\text{old}}) - \beta P(V^{\text{trial}} - V^{\text{old}}) + N \ln \frac{V^{\text{trial}}}{V^{\text{old}}} + m \ln \frac{\xi_0}{1 - \xi_0}
\]

\( m = \pm 1 \)
Physics included in our MC simulations

The plasma is completely ionized.

The degenerate, partially relativistic jellium is explicitly included in the simulations.

The ion-ion interactions are screened for partially relativistic electrons,

\[ V(r) = \frac{q^2}{r} \exp(-\kappa r) \]

Not included: quantum behavior
Our new C/O phase diagram

Allows a very accurate sampling of the phase fraction of the competing methods.

Blouin et al. 2020b

1 million core-hours

5000 core-hours
Major advantages of the Gibbs-Duhem technique

All calculations are done in the relevant statistical ensemble: phase transitions take place at constant $P$, not constant $V$

We have access to all thermodynamic properties at the phase transition (e.g., latent heat) at no additional cost (not the case with MD)
Future applications

\[ V(r) = \frac{q^2}{r} \exp(-kr/a) \]

This new simulation capability can easily be used to obtain phase diagrams of non-astrophysical systems (e.g., alloys).

We are working on adding the option of computing phase diagrams for ternary mixtures/alloys.
Future applications

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Comparison to observational data

Core crystallization leaves an imprint on the luminosity function of WDs, allowing a direct comparison to observations.

The underestimation of the crystallization pile-up may be due to the role of a 3rd minor species.

Age of the Galactic disk

Tremblay et al. 2019
Blouin et al. 2020b
\( ^{22}\text{Ne} \) in white dwarfs

\( ^{22}\text{Ne} \) makes up about 1-2% of a WD’s mass

It is produced from the leftovers of the H-burning phase

Because it has 2 excess neutrons (Z=10, A=22), the sedimentation of a given quantity of \( ^{22}\text{Ne} \) releases \( \sim 25 \) times more gravitational energy than the sedimentation of the same amount of \( ^{16}\text{O} \)
What may be going on with $^{22}\text{Ne}$

Preliminary calculations of the C/O diagram suggest that:

1. At first, there is no $^{22}\text{Ne}$ phase.
What may be going on with $^{22}\text{Ne}$

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1. At first, there is no $^{22}\text{Ne}$ phase.
2. Later, when approaching the azeotrope, the solid is depleted compared to the liquid.
3. The $^{22}\text{Ne}$-poor solid floats, leaving the $^{22}\text{Ne}$-rich liquid to the crystallization.
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1. At first, there is no $^{22}\text{Ne}$ phase.
2. Later, when approaching the azeotrope, the solid is depleted compared to the liquid.
3. The $^{22}\text{Ne}$-poor solid floats, releasing $^{22}\text{Ne}$-rich liquid to the crystal.
4. Eventually, the azeotrope is crossed, and all the remaining $^{22}\text{Ne}$ is frozen into the $^{22}\text{Ne}$-rich layer, resulting in cooling delay.
Summary

White dwarfs offer unique opportunities to study the history of our Galaxy

New observational datasets challenge our understanding of white dwarfs and call for refined physics models

We have developed an efficient and physically accurate technique to model the phase transition undergone by white dwarfs

This new technique can now be applied to other systems

Thank you! Questions?