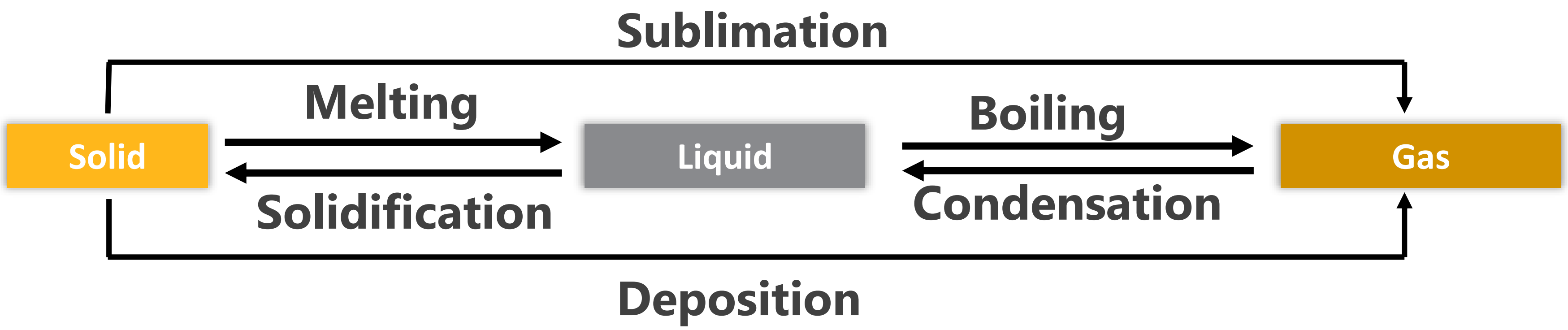
Phase Change and Enthalpy

Thermal Capacitance in Heat Transfer Analysis –
Lesson 4

Ansys

What is Phase Change?

- Matter exists in one of the three phases: solid, liquid or gas. The transition of matter from one phase to another is known as a **phase change**.



- Phase change generally occurs at a constant temperature when the pressure is constant. This constant temperature has different names based on the process, e.g., boiling point, melting point, etc.

What is Phase Change?

Melting of butter when heated

Melting of wax candle when lighted

Boiling of water

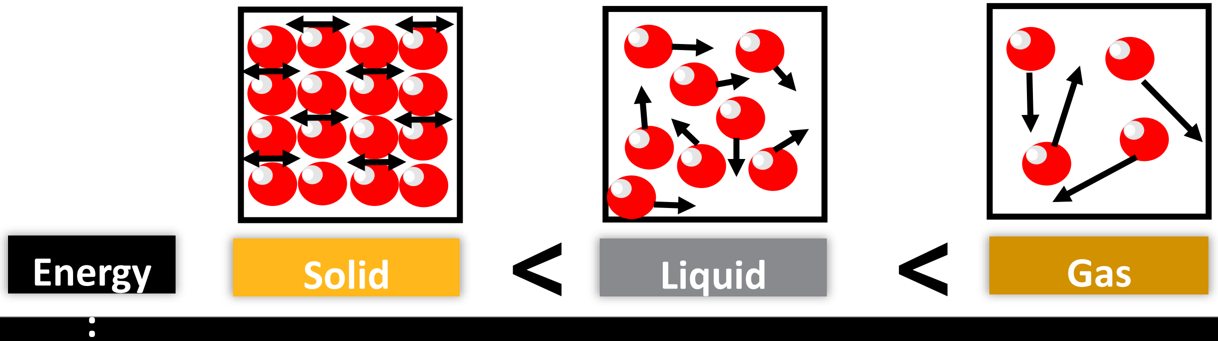
Sublimation of naphthalene balls

Sublimation of dry ice (solid carbon dioxide)

Forming of morning dew due to **condensation**

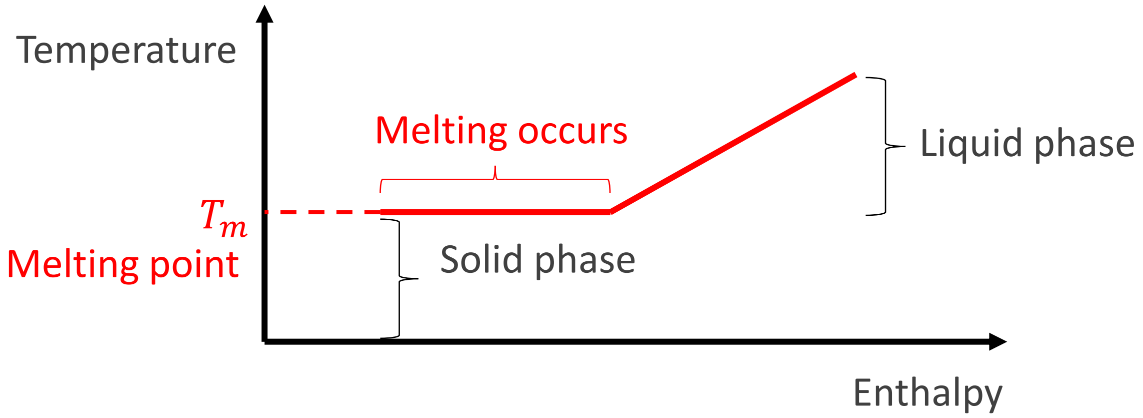
How Does Phase Change Occur?

- Gases have more energy than liquids, and liquids have more energy than solids.
- When a material is heated, the energy of its molecules increases.
- As more heat energy is added to a solid material, at a certain temperature the molecules have enough energy to overcome intermolecular forces, and transition to a liquid. This process is known as **melting** and the temperature at which this process occurs is called the **melting point**.
- Further, if we keep adding heat, at a certain temperature the molecules in the liquid will have enough energy to transition to a gas. This process is called **boiling**, and the transition temperature is called the **boiling point**.



Enthalpy

- The amount of energy required to change the phase of a material is known as the **enthalpy, H** or **latent heat** for that phase change. Its SI unit is joule.
- Heating a solid causes its molecules to vibrate more, thereby increasing the temperature of the solid (as predicted by its specific heat).
- When the temperature of the solid reaches its melting point, adding more heat does not change the temperature because all the heat goes into melting the solid. Thus, phase change generally occurs at a constant temperature.
- Few exceptions exist, e.g., amorphous solids do not have ordered internal structure, and hence do not have a sharp melting point.



Enthalpy

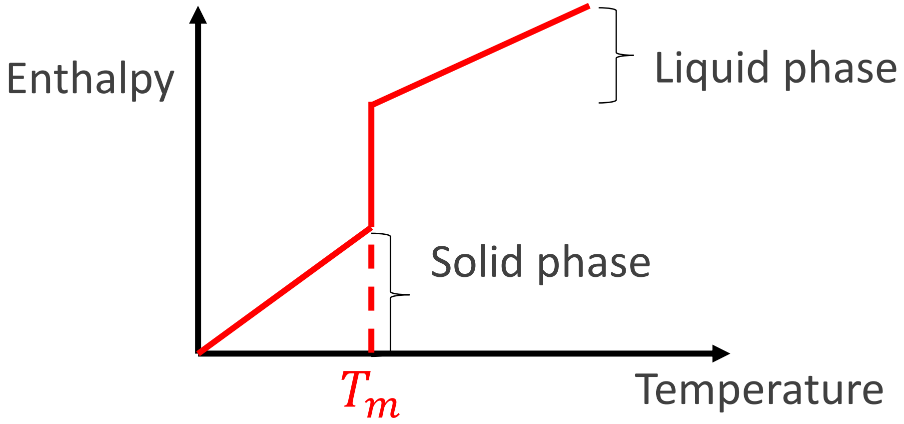
- The amount of heat required to melt the solid completely is known as the **enthalpy of melting** or **latent heat of melting**.
- The enthalpy of solidification is numerically equal to the enthalpy of melting. But the enthalpy of melting is positive (heat is added to the system), while the enthalpy of solidification is negative (heat is removed from the system).
- The temperature at which phase change occurs in a given material depends on the pressure.
- For example, water boils at 100^0C at atmospheric pressure, but boils at 120^0C in a pressure cooker due to higher pressure. Thus, food cooks faster in a pressure cooker.

Simulating Phase Change

- Enthalpy is an additional material property that needs to be defined when simulating melting or solidification.
- Generally, in textbooks, enthalpy is defined as the energy absorbed or released by a body to undergo phase change.
- But in simulations, this definition is modified to be the energy absorbed by a "unit volume" of a body (i.e. it has dimensions of energy/volume).
- Enthalpy can be calculated from specific heat capacity, c, and density of material, ρ, using:

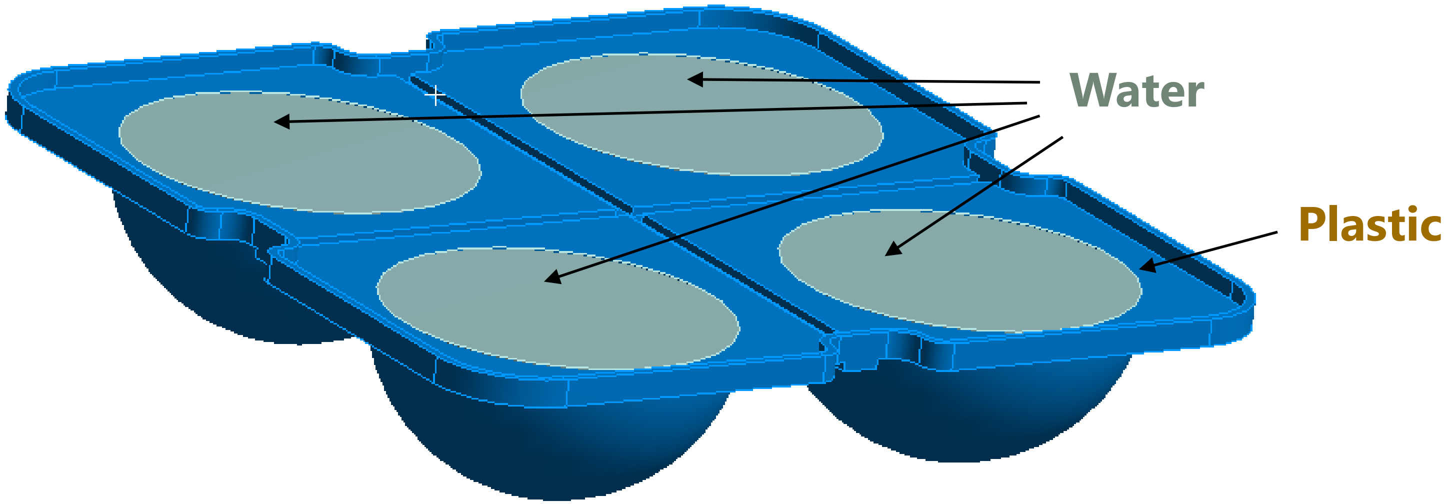
$$H = \int \rho \, c(T) dT$$

- But for accuracy, we define an enthalpy curve.



Simulating Freezing of Water to Ice – Geometry

- Let us simulate the freezing of water to ice in a freezer. Let's assume that the water is initially at 10^0C. The freezer is maintained at a constant temperature of -5^0C. The freezing point of water is 0^0C.



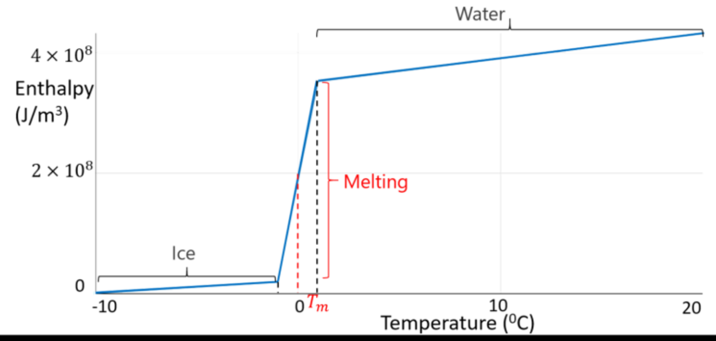
Simulating Freezing of Water to Ice – Material Properties

- We first need to define an enthalpy curve for water, using the data on the right.
- Let's say the enthalpy is 0 at -10^{0}C. Instead of a distinct melting point at 0^{0}C, let's assume melting starts at -1^{0}C and ends at 1^{0}C (to avoid abrupt, steep changes in enthalpy).

Property	Value
Melting point	0^{0}C
Density	997 kg/m^3
Solid specific heat (for ice), c_s	2108 J/kg-^{0}C
Liquid specific heat (for water), c_l	4220 J/kg-^{0}C
Enthalpy of melting, ΔH_m	334000 J/kg

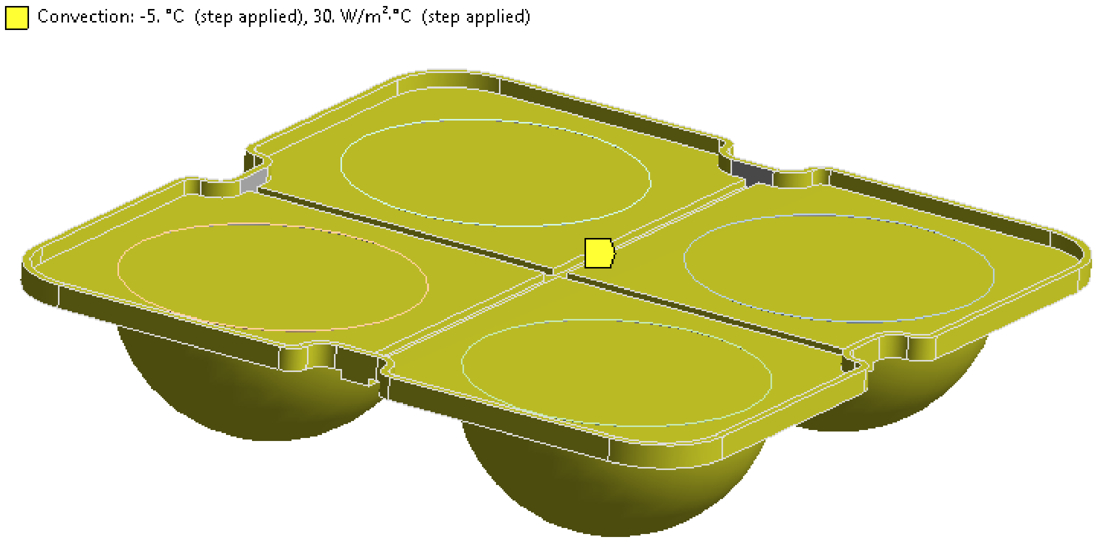
- $H_{T=-1^0C} = H_{T=-10^0C} + \rho c_s \Delta T = 0 + 997 \times 2108 \times 9 = 18915084 \text{ J}/m^3$
- $H_{T=1^0C} = H_{T=-1^0C} + \rho \Delta H_m = H_{T=-1^0C} + 997 \times 334000 = 351913084 \text{ J}/m^3$
- $H_{T=20^0C} = H_{T=1^0C} + \rho c_l \Delta T = H_{T=1^0C} + 997 \times 4220 \times 19 = 431852544 \text{ J}/m^3$

T (^{0}C)	H (J/m^3)
-10	1e-5
-1	18915084
1	351913084
20	431852544



Simulating Freezing of Water to Ice – Boundary Conditions

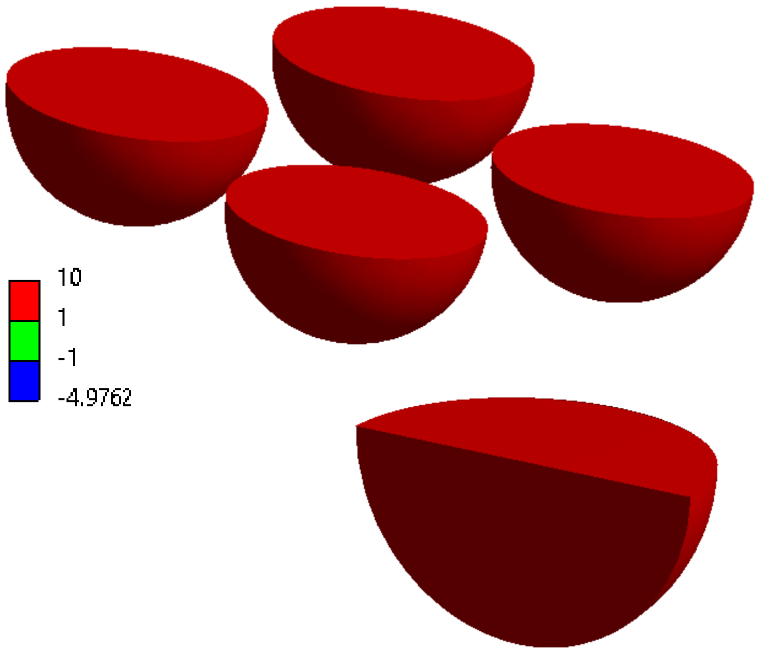
- The initial temperature of the water and the ice tray is defined to be 10^0C.
- We define a step which is 10,000 s long (166.6 minutes). The convection boundary condition is defined on the surfaces of the ice-tray and the water that are in contact with the cold freezer air. We assume a film coefficient of 30 $W/m^{2}\cdot{}^0C$. The ambient temperature of the freezer is assumed to be -5^0C.



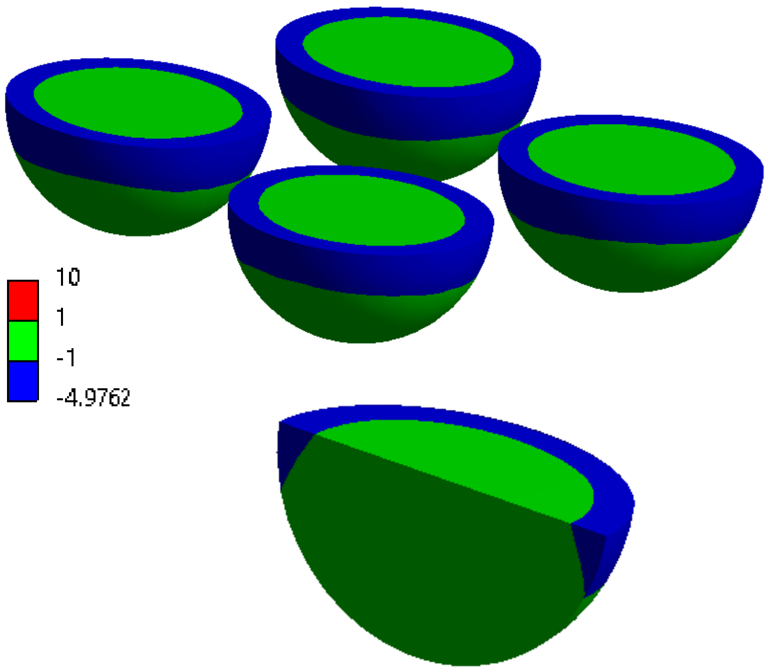
Simulating freezing of water to ice – results

Temperature distribution at different times. Red = liquid, green = transition, blue = solid.

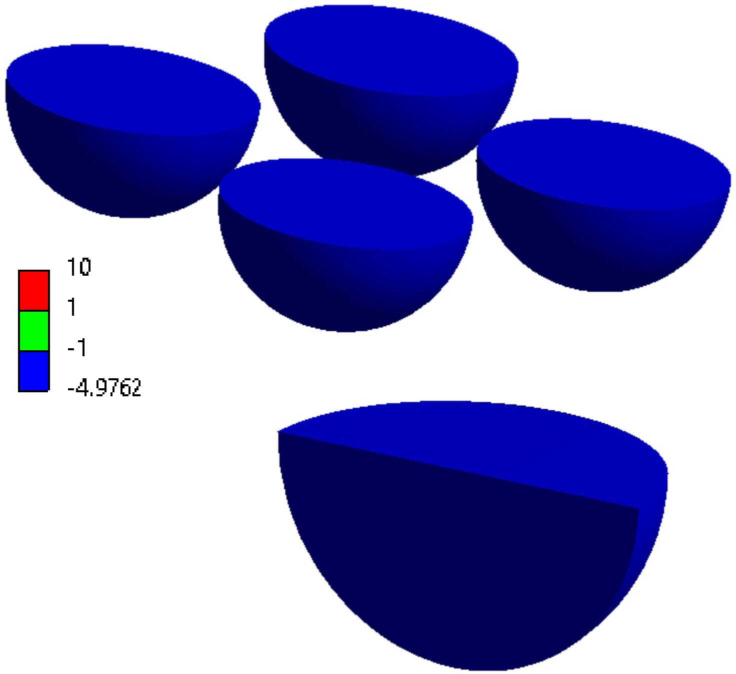
t = 100 s – Water is in a liquid phase



t = 4210 s - Transition between liquid and solid phase

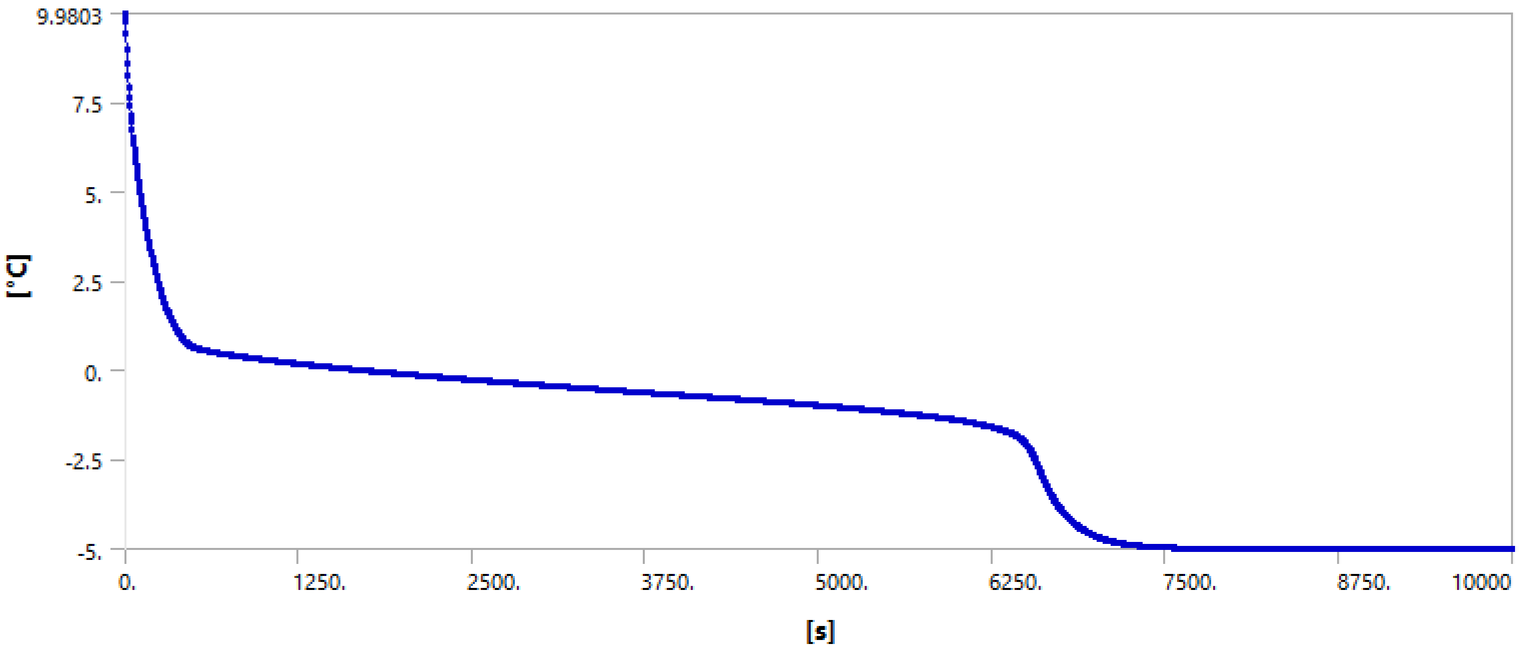


t = 6620 s (1 hr 50 min) - All water solidified into ice.

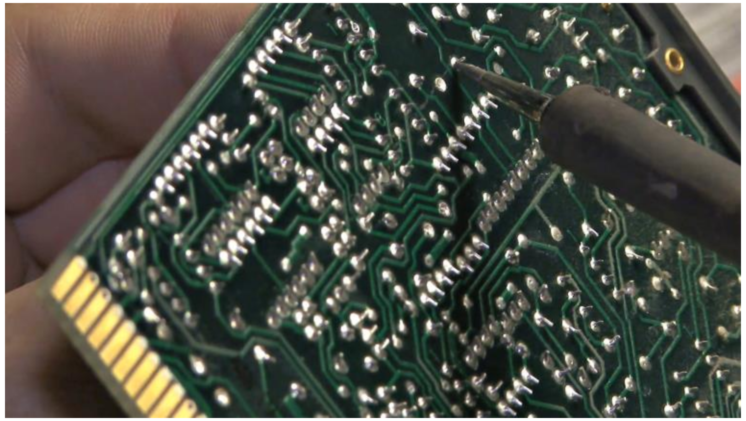


Simulating Freezing of Water to Ice – Results

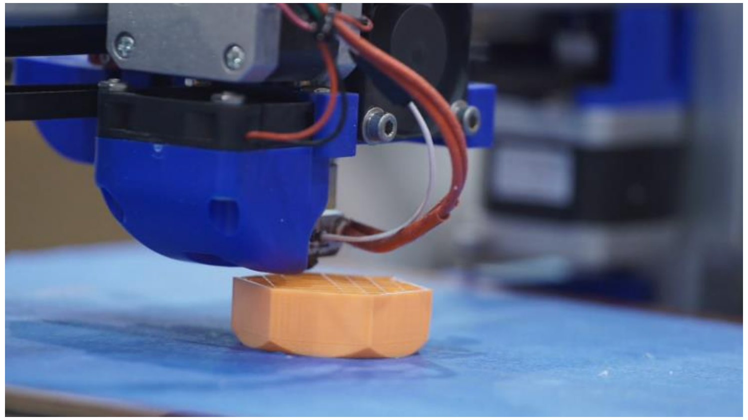
If we plot the variation of average temperature of water with time, we find that the temperature remains almost constant at 0^0C when the water undergoes freezing. Thus, heat removed from water during this time does not reduce the temperature of the water but is in fact spent in transforming the water to ice.



Applications of Melting and Solidification in Industry



Solder is melted and solidified quickly to connect various electronic parts.



3D printing involves depositing material in liquid phase layer-by-layer, and allowing it to cool down to form complex solid shapes.

Casting is a process in which molten metal in liquid phase is poured in a mold and cooled to get a solid body with the desired shape.

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