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Theory of Liquid Crystallization

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Abstract

In actual fact, most basic metal and base materials are made by liquid crystallization. Study on the crystallization process includes the main tasks are: thermodynamic conditions of crystallization; The basic stages (processes) of crystallization; Characteristic factors for crystallization and post-crystallization; Quality of post-crystalline materials and measures to improve the quality of materials; Dynamics of crystallization; Actual composition and defects may appear in the product after crystallization.

Keywords: material, liquid metal

Introduction

Previously, in the old opinion, the liquid state of the metal was considered to be close to the vapor state. At present, however, with the development of science, by applying high-tech research methods such as Roughens beam analysis, electron rays, electron microscopes, etc., Liquid has some of the following characteristics:

- At near crystalline temperature, liquid metal volume is approximately equal to solid metal volume.
- The liquid density of the liquid metal is approximately equal to the isoelectric constant of the metal in the solid state.
- Mild melting (from solid to liquid) is much smaller than vaporization (from liquid to vapor)
- Both liquid metal and solid state metal conduct electricity and conduct heat well.

From the above, we can draw some basic conclusions: The distance between metal atoms in liquid and solid states is approximately the same (due to their nearly identical volume), so there is a stable arrangement of the molten metal atoms. The heat oscillation of the metal atoms around the equilibrium position in the two states is nearly identical (due to their own specific heat), so that the stability of the atoms is nearly identical. Liquid metal is still present in liquid metal (expressed through conductivity). So we can conclude that: In liquid metals, atoms retain only near order but do not keep as far away as solid metal.

Energy condition of the crystallization process

As we all know, all physical systems tend to exist in states with lower free energy levels. With the crystallization process, most of the liquid metal crystallization is in atmospheric atmospheric pressure and can be considered as a process of equilibrium. The free energy of the system (Gibbs energy) is calculated by the expression:

$$G = H - T.S \quad (2.1)$$

Where

- G: free energy of the system;
- T: Temperature ($^{\circ}$ K)
- H: Enthalpy of the system;
- S: Entropy of the system.

$$\text{Free energy variable of the system: } dG = dH - T.dS - S.dT \quad (2.2)$$

Because of the isotropic ($P = \text{const}$) process, we have:

$$dH = C_p.dT \quad (2.3)$$

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Replace (2.3) with (2.2) we have:

$$dG = -S.dT = - \left[\int_0^T C_p \cdot \frac{dT}{T} \right] dT \tag{2.4}$$

$$G = G_0 - \int_0^T \left[\int_0^T C_p \cdot \frac{dT}{T} \right] dT \tag{2.5}$$

From equation (2.5), we have the graph of free energy change of liquid phase and solid phase as shown in Fig 1.

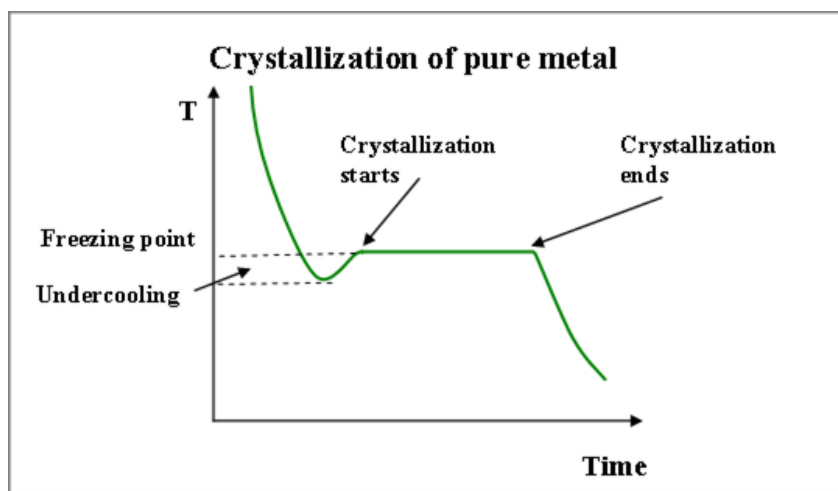
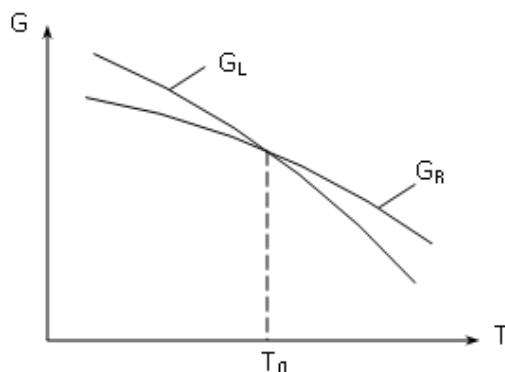


Fig 1: Graph of free energy changes of solid and liquid metals by temperature

On the graph we see two curves intersect at a temperature point T₀. From this graph we find that: When the system temperature is less than T₀, then the free energy of the solid phase is smaller than the liquid phase, so the solid state will be stable and the metal will exist in solid state. Conversely, when the temperature is greater than T₀, the free energy of the liquid phase will be smaller than that of the solid phase and hence the liquid state becomes more stable, the metal will remain liquid. When the metal temperature T₀ exists in equilibrium state. Thus, to the process of crystallization of liquid metal must have conditions:

$$\Delta G = G_s - G_l < 0$$

Where:

G_s is solid energy

G_l is liquid energy

Temperature T₀ is called the crystalline theoretical temperature of the metal, at this temperature there exists a state of equilibrium between the liquid phase and the solid phase, has not occurred crystallization, so many solid particles appear. then there is the dissolution of liquid metal back to solid particles.

At temperature T₀ we have:

$$G_l = G_s \tag{2.6}$$

$$H_l - T_0.S_l = H_s - T_0.S_s \tag{2.7}$$

$$H_s - H_l = T_0 (S_s - S_l) \tag{2.8}$$

$$T_0 = \frac{\Delta H}{\Delta S} \tag{2.9}$$

ΔH: The thermal difference between the solid state and the liquid state of the primary metal is the melting point of the metal and is denoted as L_{m/c}. Thus,

$$T_0 = \frac{L_{m/c}}{\Delta S} \tag{2.10}$$

The theoretical crystalline temperature difference and the crystalline T_k are called cool degrees

$$\Delta T = T_0 - T_k \tag{2.11}$$

Thus crystallization conditions occur only when there is too much cold ΔT > 0, which means that the rod must be slightly smaller than glowing. Actually, metals can crystallize at different temperatures ie with different degrees of cooling

Germination process

When crystallized, it is not instantaneous that the entire volume of liquid metal goes into solid state but goes through different stages over time. Initially in the liquid

metal there was the appearance of the first solid particles, which did not dissolve back to the liquid metal. This is called germination. The germination process comes in two basic forms: spontaneous (synchronous) or parasitogenic (spherical) germination.

Create sprouts spontaneous

Sprout sprouts are sprouts produced from the liquid metal itself, unaffected by external factors. The process of spontaneous sprouting occurs when a group of atoms is ordered, fixed to form the lattice structure of the same type as that of the crystal lattice. When there is a solid element in the liquid metal, we see two opposite changes in energy:

- The decrease in energy when a liquid phase volume becomes solid (due to crystallization at a temperature lower than T_0 , the free energy of the solid phase is smaller than the liquid phase).

- When the solid phase is created, a new surface and surface energy appear, resulting in increased system energy. The free energy variable of the system is:

$$\Delta G = -\frac{4}{3}\pi r^3 \cdot L_{n/c} \cdot \frac{\Delta T}{T_0} + 4\pi r^2 \cdot \sigma \quad (2.12)$$

Wherr

σ : Unit surface tension of the seed surface.

From Equation (2.12) we can draw a graph describing the energy variation of the system according to the change of the newly created solid-phase radius (Fig. 2). From the graph we see that there exists a r_{th} value at which the energy change value ΔG is maximized. Therefore, when the sprouts produced have smaller r_{th} will not develop, but dissolved back to liquid metal. Only sprouts with a radius greater than r_{th} will continue to grow, gradually replacing the liquid phase to perform the crystallization.

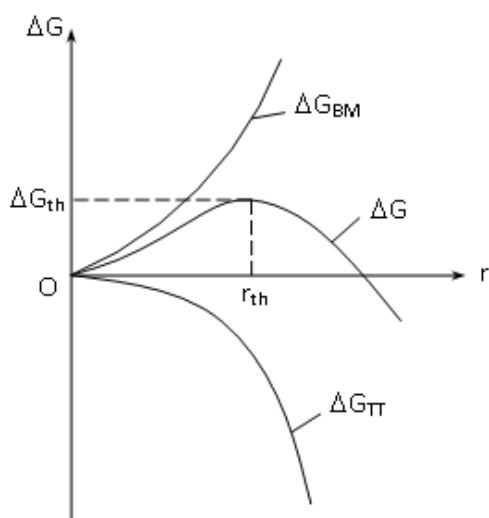


Fig 2: Free-energy variation of the system according to the new sprout radius

We can calculate the r_{th} radius as follows:

$$\begin{aligned} \frac{\partial(\Delta G)}{\partial r} \Big|_{r=r_{th}} &= 0 - 4\pi r_{th}^2 \cdot L_{n/c} \cdot \frac{\Delta T}{T_0} + 8\pi r_{th} \cdot \sigma = 0 \\ \Leftrightarrow 4\pi r_{th} \left(2\sigma - r_{th} \cdot L_{n/c} \cdot \frac{\Delta T}{T_0} \right) &= 0 \Leftrightarrow r_{th} = \frac{2\sigma \cdot T_0}{L_{n/c} \cdot \Delta T} \end{aligned} \quad (2.13)$$

From the expression (2.13) we see that the value of the radius of the sprout is inversely proportional to the degree of coolness of the crystalline ΔT . As the larger the ΔT value (ie the smaller the crystallization temperature), the smaller the r_{th} will be and therefore the faster the germination, the more likely the germination to develop is with a small radius. Than. In addition, the critical radius value depends on the physical properties of the crystalline metal itself. The expression (2.13) also confirms that, at the temperature T_0 ($\Delta T = 0$) the crystallization process cannot occur due to $r_{th} = \infty$. Thus, the energy needed to generate r_{th} is:

$$\Delta G_{th} = \frac{1}{3} 4\pi r_{th}^2 \cdot \sigma = \frac{1}{3} \Delta G_{b\grave{e} m\grave{a}t} \quad (2.14)$$

This energy source is based on the three energy dynamics of the system, the energy value of the molten metal when crystallized is to be understood as the mean value. The energy of the small volume varies at different times of change, possibly greater or less than the mean. If more energy is added to the three energy dynamics to provide the missing energy to the surface, then the germination will occur.

Create parasitic germs

Spore germs are germs created on the basis of "available solid particles" in the liquid metal. The term "snake seed available" includes the following basic elements:

- Formation of liquid metal when crystallized.
- Impurities are difficult to melt in liquid metal (eg Al_2O_3 , Cr_2O_3 , in liquid metal).
- Wall dust mixed in liquid metal.

With the emergence of solid particles available, the free energy change in germination in this case has its own characteristics. Suppose on the surface of a solid particle that a nucleus is created that has the form of a cone with radius r . The angle ϕ is the contact angle between the sprout and the solid surface.

$$r_{th} = \frac{2\sigma_{ML} \cdot T_0}{L_{n/c} \cdot \Delta T}$$

And the energy needed to create the parasitic spike has a critical radius:

$$\Delta G_{th} = \frac{1}{3} C \cdot \sigma_{ML} \cdot 4\pi r_{th}^2$$

The above expression shows that the energy needed to create the parasitic sprout depends on the angle ϕ . And only the energy needed to generate sprouts is by the factor $C = 2-3 \cos\phi - \cos^3\phi$

We find that $\cos\phi$ can receive values from -1 to +1, to show the effect of angle ϕ we consider the following cases: When $\cos\phi = -1$, angle $\phi = 180^\circ$, the coefficient $C = 1$ is the spherical sphere, then the sprouting process returns to the sprouting sphere and the role of the solid in the crystallization process is No longer, because then the seed formation on the solid phase will have higher energy when the germination in the liquid phase.

When $\cos\phi = 1$, angle $\phi = 0^\circ$, coefficient $C = 0$, ie $\Delta G_{th} = 0$, this is the ideal case where the sprouting process is much more profitable than that of spontaneous sprouting.

In all other cases where $\cos\phi$ is always greater than -1 and less than 1, the C factor is always greater than 0 and less than 1. The energy that produces the parasite will be smaller than that of the sprout. Then the surface of the solids available facilitates faster crystallization.

Conclusion

The germ development process is the development of the size of the solid particles to gradually occupy the volume of the liquid phase. There are two theories about the germination process: the germination mechanism grows under incomplete atomic layers and the germ grows along the helix. Incomplete atomic layer is the part where crystalline structure occurs and is lost in liquid metal near crystalline temperature. In the solid phase always exists deviation containing the twisted order? Because the crystal contains a helix deviation, the surface is orthogonal to the axis of the deviation in the form of a helix, on which there are already available levels acting as incomplete atomic layers. Both germination mechanisms have their own values and speak of two real possibilities of crystal growth. Their similarity is that on the rising crystalline surface there must be levels to the atom from the liquid phase. There are also two real possibilities in the crystallization process.

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