An Analytical Study of Thermal Waves Facing the Austenitic Steel

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Abstract

Iron (Fe-C) being the most acceptable container material exposed to higher temperature ranges. This study is based on the Austenite Face Centered Cubic structure of Iron. The crystal structure of the material, the wavelength of the thermal radiation, the packing factor of the FCC crystal structure, the thermal conductivity, the free electron model are main concepts taken into consideration. The thermal behaviour of the material is explained analogous to the light wave of reflection, absorption and refraction.

1. Introduction

A Face Cubic Centered unit cell is taken for the case study. Iron atom is considered to simulate the austenite iron FCC form. Since in most of the cases the reactor vessel is made out of iron (Fe), which is a very robust material at higher working temperature. This study aims to find the way of heat transfer within the solid. Considering metal as a cloud of electrons with nucleus and applying the temperature gradient across the sample cube and analyses the result.

1.1 Austenitic Steel

Austenite is an interstitial solid solution of carbon in face cubic centered gama-iron. This phase can dissolve up to 2% of carbon at 1147 degree centigrade. The phase is stable only above 727 degree centigrade. This is soft, ductile, malleable, and non-magnetic (paramagnetic) phase.

- Body Centered Cubic (2 atoms/cell)
- Face Centered Cubic (4 atoms/cell)

Figure 1.

$$
a_{\text{bcc}} = 4R/\sqrt{3}
$$

$$
\rho_{\text{bcc}} = 2x\text{Atomic Weight}(\sqrt{3})^3/\text{N}(4R)^3
$$

 $a_{\text{fcc}} = 4R/\sqrt{2}$ $\rho_{\text{fcc}} = 4 \text{xAtomic Weight}(\sqrt{2})^3/\text{N}(4\text{R})^3$ $(\rho_{\text{fcc}} - \rho_{\text{bcc}})/\rho_{\text{bcc}} = (4\sqrt{2} - 3\sqrt{3})/3\sqrt{3} \times 100 = 8.89\%$

Thus it is clear that there is an increase in density of 8.89% when iron phase changes from BCC to FCC. This result in decrease in specific volume.

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Figure 2.

1.2 Analysis

Considering sample cube with appropriate number of iron FCC unit cells.

1.2.1 At X=0

Figure 3.

Total surface area = $a^2 = (2\sqrt{2} R)^2 = 8R^2$ Surface area unoccupied = $8R^2$ - $2\pi R^2$ = 1.72 R^2 Surface area occupied = $(8-1.72)R^2 = 6.28 R^2$

1.2.2 At X=a/2= √2R

Figure 5.

Surface area unoccupied = $8R^2 - 2\pi R^2 = 1.72 R^2$ Surface area occupied = $(8-1.72)R^2 = 6.28 R^2$

1.2.3 At X=a = 2√2R = 2.828R

Surface area unoccupied = $8R^2 - 2\pi R^2 = 1.72 R^2$ Surface area occupied = $(8-1.72)R^2 = 6.28 R^2$

Up till now the ratio of occupied to unoccupied remains same which is 3.65 with changing 'a'

1.2.4 At X=0.414R

Figure 7.

Area $= \pi R^2 - \pi (0.4R)^2$ $= 0.84 \pi R^2$ The total surface occupied at X=0.414R is $= 2x0.84\pi R^2$ $= 5.27R^2$ The total surface area unoccupied become $= 8R^2 - 5.27R^2$ $= 2.73R^2$

The total surface area exposed inside the unit cell $= 4x2\pi R^2 + 4\pi R^2$ $=$ 37.68 R^2

The total surface area unoccupied for unit cell in all its six surfaces

$$
= 6x1.72R^2
$$

$$
= 10.32R^2
$$

Thus approximately the internal surface area exposed = 3 times the surface area unoccupied at outer surface of the cubic unit cell.

1.3 Application

Appling the Newton's law of cooling and Fourier's law of heat conduction across the FCC unit cell.

Figure 8.

Radius of iron atom is taken as $= 126 \times 10^{-12}$ m Forming the sample piece by considering 10^8 FCC unit cells in an array made out of one side of the cube which results a cube of 3.563 cm of each side.

> $a = 2\sqrt{2xR}$ m $= 2x1.414x126x10^{-12}x10^8$ m $= 3.563$ cm

Thus the sample cube selected is of side 3.563 cm. 108 units selected just to reach to an optimum value of sample cube.

Applying the conditions for heat transfer Number of iron atom in 3.563 cm side cube is $= 4x10^8x10^8x10^8$ $=4x10^{24}$ atoms.

Here number 4 is for number of atoms in the unit cell present.

$$
q=h_i^* A^*(300-T_1)
$$

(300-T_1)/q=1/h_i.A_{occupied}
(1)

$$
q = -k^* A^* (T_2 - T_1)/a
$$

\n
$$
(T_1 - T_2)/q = a/k^* A_{exposed}
$$

\n
$$
q = h_0^* A^* (T_2 - 30)
$$
\n(2)

$$
(T_2 - 30)/q = 1/h_o * A_{\text{occupied}} \tag{3}
$$

from equation
$$
1, 2, 3
$$
 we have

$$
(300-30)/q=1/h_{i}A_{\text{occupied }+}a/kA_{\text{exposed}}+1/h_{o}A_{\text{occupied}}
$$

Assumption: Consider all the surrounding four surfaces to be insulated that is all the energy what so ever entering will be going out via the surface at

 $x = a(3.563cm)$. $270/q = 240.719$ $q = 1.12168$ watts Applying the $E = 1/2mv^2$ $V = \sqrt{(2E/m)} = \sqrt{(2x1.12168)/(4x10^{24}x55.84)}$ Velocity = 0.10021×10^{-12} m/s Time = 2 x radius/velocity $= (2x126x10^{-12}m)/0.10021x10^{-12}m/s$ $= 2x1257.35$ seconds

Thus 1.1268 watts of energy will take 42 minutes to cross an atom of FCC unit cell.

This result reflects that heat wave or heat energy is not travelling within a solid classically.

Appling the Einstein's energy conversion formula I reach the value

```
\lambda = hc/E
```

```
=[6.626x10^{-34} Js x0.0021x10^{-12} m/s]/1.12168 J
```
- λ =hc/E
	- $=[6.626 \times 10^{-34}$ Js $x3 \times 10^8$ m/s]/1.12168 J

 $= 17.721 \times 10^{-26}$ m

2. Result

Intensity = power/area = energy/time x area = (energy x length)/time x volume

```
 = (energy x velocity)/volume
Intensity = (1.12168 \times 0.10021 \times 10^{-12})/(3.563x10^{-2})^3= 2485.03535 watts/m<sup>2</sup>sec
since c = v\lambda = \lambda/T = \lambda^2 2\pi/T^2 2\piand \omega = 2\pi/T; v = A \omegaω = c<sup>2</sup> 2π/λ =3*108
*2*3.14/17.721x10-26
    = 1.0631^{\circ}10^{34}rad/sec
A = v/ \omega = 0.10021 \times 10^{-12} / 1.0631^* 10^{34}= 0.094262^{*}10^{-46}
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Since the maximum space available between the fcc iron atoms is of the order of 10-14 m and the amplitude is of the order of 10-46 m. This clearly reflects that about 10^{32} waves can pass through the individual unit cell. and thus supports the wave nature of heat.

3. References

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