Modelling of Solute Segregation in Ti-6Al-4V Produced by Selective Laser Melting

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1. Introduction

Titanium alloys are used in aero engines and body implants. If they can be additively manufactured while keeping desired properties, the cost of production would be reduced significantly, opening up the markets for cheap aero engine repairs. Also, additive manufacturing allows manipulating and printing of lattice structures, which could have stiffness matching actual bones. By printing on a heated powder bed, the heat treatment step in the production line could be removed, shortening the production time.

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This project was designed to examine how solute segregation could affect the microstructures of additively manufactured Ti-6Al-4V samples and thus, to understand how properties could be optimised. The results obtained could also be applied to many different alloy systems, such as steels, which exhibit similar solute segregation behaviour at higher temperatures.

2. Background

Solute segregation was observed at crystal defects of Ti-6Al-4V samples produced by selective laser melting on a heated base plate. For base plate temperature of 570 ˚C, segregation of V was observed at dislocations. This behaviour was observed for the first time, and its mechanisms are examined.

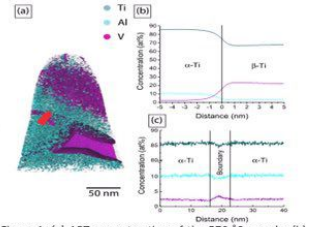

Figure 1: (a) APT reconstruction of the 570 ˚C sample. (b) 1D concentration profile across grain boundary. (c) 1D concentration profile across dislocation [1].

3. Dislocation and Diffusion

Solute segregation can only happen when dislocation velocity is slow, so that the solute cloud can diffuse quickly enough to move along with the dislocation.

Dislocation velocity: $v = \frac{\varepsilon\,(strain\ rate)}{\rho b}$

Diffusion coefficient of V in alpha Ti:

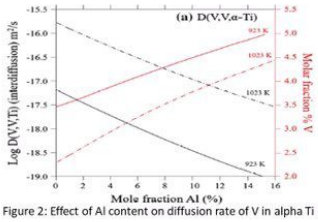

Figure 2: Effect of Al content on diffusion rate of V in alpha Ti [2].

$$D = D_0 \times e^{-\frac{Q}{RT}}$$

$$D(Al) = 10^{-0.12Al + \log D}$$

Relationship between dislocation velocity and diffusion coefficient during solute segregation:

$$v = v_d \frac{\tau b^4}{kT} \exp\left(-\frac{U_d}{kT}\right) = D\frac{\tau b^2}{kT}$$

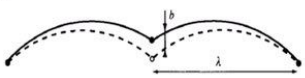

Figure 3: Schematic description of the diffusion-controlled glide of a dislocation pinned by a row of solute atoms [3].

v	3.0566×10^{-9} m/s
D (theoretical)	5.8701×10^{-19} m^2/s
D2 (experimental)	1.8104×10^{-20} m^2/s

At the dislocation velocity calculated, the experimental value of the diffusion coefficient is close to the theoretical value. Thus, segregation of V to the dislocation is expected in our sample.

4. Nucleation Model

Heterogeneous nucleation of β phase in α matrix at dislocations [4]:

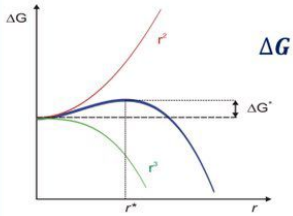

Figure 4: Graph of change in Gibbs free energy versus radius of the nucleus.

$$\Delta G = \frac{4}{3}\pi r^3 \Delta G_v S + 4\pi r^2 \gamma S + \frac{4}{3}\pi r^3 \Delta G_{el} S$$

$$S(\theta) = \frac{1}{2}(2 + \cos\theta)(1 - \cos\theta)^2$$

$$\cos\theta = \frac{1}{2}\frac{\gamma_{AA}}{\gamma_{AB}}$$

Interface energy:

By assuming isotropic incoherent interface [5]

	570 ˚C
γ_β (mJ/ m^2)	866.3
γ_α (mJ/ m^2)	1436.4
$\gamma_{\alpha\beta}$ (mJ/ m^2)	744.6

$$\gamma_\beta = (449 \pm 10) - (0.385 \pm 0.096)(T - T_s)$$

$$\gamma_\alpha = (2200 \pm 164) - (1.48 \pm 0.20)T$$

$$\gamma_{\alpha\beta} = (1041 \pm 85) - (0.57 \pm 0.10)T$$

Volumetric driving force:

The Gibbs free energy of each phase is calculated using the equation below [6]:

$$G^\beta = G^0 + G^{ideal} + G^{XS}$$

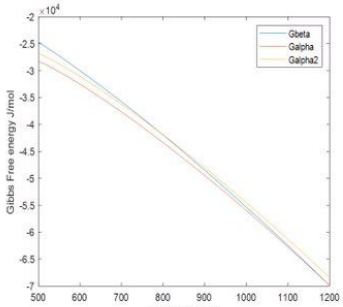

Figure 5: Variation of Gibbs free energy with temperature.

Below β transus (980K), alpha phase is more stable than beta phase, making nucleation of beta phase unfavourable.

Presence of the dislocation strain could raise the Gibbs free energy of alpha phase [7]:

$$\Delta G_s = \varepsilon \rho V_m$$

Parameters	570 ˚C
G_α	-4.2969×10^4 J/mol
G_β	-4.1522×10^4 J/mol
$G_\beta - G_\alpha$	1.4465×10^3 J/mol
ρ1 ($G_\beta = G_\alpha$)	6.2377×10^{17} /m^2
ρ2 (experimental)	1.37×10^{14} /m^2

The Gibbs free energy of alpha phase increases with increasing dislocation density. The dislocation density obtained experimentally was not high enough to provide a negative driving force.

5. Conclusions

- Solute segregation of V at dislocations of alpha grains was observed as the dislocation velocity is comparable with the diffusion rate of V in alpha Ti at 570˚C.
- This segregation phenomenon at the given conditions would not cause the nucleation of beta phase in alpha matrix as negative driving force could not be established.

6. References

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