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INVESTIGATION OF THERMAL CONDUCTIVITY IN ADVANCED METALLIC MATERIALS VIA COMPUTATIONAL FLUID DYNAMICS

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ABSTRACT

This study investigates the transient thermal behavior of Ti6Al4V alloy using computational fluid dynamics (CFD) simulations. The primary objective is to characterize the alloy's heat-conduction performance under controlled thermal-loading conditions. A dual-scale modeling approach was employed, combining a simplified body-centered cubic (BCC) lattice structure to represent the β-phase and a macroscopic solid domain to simulate the bulk material response. The simulations were performed over a 10-minute interval, with thermal data extracted at 1-, 3-, 5-, and 10-minute time steps. The results indicate delayed, uneven heat propagation in Ti6Al4V, attributed to its intrinsically low thermal conductivity (6.5 W/m·K). The findings provide insight into the alloy's thermal limitations, particularly in applications requiring efficient heat dissipation. The study demonstrates the potential of CFD as a predictive tool for evaluating thermal performance in advanced metallic materials.

KEYWORDS: thermal conductivity, Ti6Al4V, CFD, transient heat transfer

1. Introduction

Ti6Al4V is one of the most widely used titanium alloys in high-performance engineering sectors such as aerospace, biomedical implants, and additive manufacturing, due to its excellent strength-to-weight ratio, corrosion resistance, and biocompatibility [1-4]. However, its relatively low thermal conductivity - typically between 5 and 7 W/m·K - poses challenges in applications requiring efficient heat dissipation [5-7]. This limitation becomes critical in processes like laser powder bed fusion (LPBF), where high thermal gradients can lead to undesirable microstructures, residual stresses, and thermal distortion [8-10]. Notably, experimental studies have revealed significant discrepancies in thermal conductivity between bulk and powder forms of Ti6Al4V. For example, Saeidi *et al.* reported ~0.13 W/m·K for powder, compared to ~5.4 W/m·K for bulk material, emphasizing the effects of porosity and contact resistance [3, 11, 12]. The influence of phase composition is also important, as Ti6Al4V exhibits a dual-phase (α + β) structure. The β-phase, typically modeled using a BCC lattice, shows directional heat transfer behavior, which can be impacted by grain morphology and crystallographic orientation [6, 13]. Such microstructural factors play a significant role in thermal anisotropy.

Computational fluid dynamics (CFD) has emerged as a valuable tool for modeling the thermal response of Ti6Al4V under various boundary conditions. CFD DEM semi-coupled simulations have been employed to model powder–build interactions, melt pool formation, and porosity development in LPBF processes [6, 14-16]. These models help in optimizing process parameters such as scan speed and preheating temperature, ultimately enhancing component quality [9, 6, 17]. Furthermore, powder properties such as particle size, shape, and packing density significantly affect the effective thermal conductivity, especially in electron beam powder bed fusion (EB-PBF) processes [18].

Despite the growing body of literature, most studies integrate convective and radiative effects, which obscure the alloy's intrinsic conductive properties. To bridge this gap, the present study

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employs CFD simulations to investigate transient thermal conduction in Ti6Al4V under strictly conduction-dominated conditions. A dual-scale modeling approach is used: a macroscopic solid domain for bulk behavior, and a microstructural BCC lattice for directional heat transfer in the β-phase. This framework aims to isolate material-specific effects and provide insights for the design of thermally optimized components using Ti6Al4V. The implementation of computational fluid dynamics (CFD) in this study is justified by its demonstrated capability to accurately model transient heat conduction phenomena in metallic materials. As a numerical technique, CFD offers a rigorous and flexible framework for solving the governing heat transfer equations under well-defined boundary conditions, thus enabling detailed simulation of thermal diffusion across both macroscopic domains and microstructural representations.

In the specific case of Ti-6Al-4V, a dual-phase alloy characterized by notable thermal anisotropy, CFD facilitates the quantitative assessment of directional heat conduction as influenced by crystallographic architecture and phase morphology. This is particularly relevant when analysing idealized body-centered cubic (BCC) lattice configurations that approximate the behavior of the β-phase. Unlike analytical or empirical approaches, CFD provides enhanced spatial and temporal resolution, which is important for capturing multi-scale thermal transport phenomena. Furthermore, it allows the explicit isolation of conduction mechanisms by excluding convective and radiative contributions - thereby offering a more intrinsic evaluation of the material's conductive properties. Considering the inherent difficulties associated with experimental characterization of heat flow in complex microstructures, CFD emerges as a powerful predictive tool for advancing both scientific insight and thermally optimized component design.

2. Experimental Procedure

To investigate the transient thermal conduction behavior of Ti6Al4V, a series of computational fluid dynamics (CFD) simulations was performed using two complementary geometric models: a macroscopic solid block and a microstructural lattice structure representing the β-phase. This dual-scale approach was designed to capture both global and directional thermal diffusion phenomena specific to the alloy. The macroscopic model consisted of a solid rectangular domain with dimensions 100 mm × 300 mm × 10 mm, intended to approximate bulk material behavior under thermal loading. In parallel, a simplified body-centered cubic (BCC) lattice with dimensions 4 mm × 4 mm × 3 mm was constructed to mimic heat transfer pathways within the β-phase of the alloy. This structure was used to explore localized anisotropic conduction effects resulting from the crystallographic configuration of the β-phase.

Material properties were defined based on literature values validated by experimental measurements. Ti6Al4V was assigned a density of 4410 kg/m^3, a thermal conductivity of 6.5 W/m·K, and a specific heat capacity of 326 J/kg·K. These values ensured realistic thermal behavior within the simulation environment and enabled time-accurate transient analysis.

The simulation domain was initialized with an ambient temperature of 20 °C. A thermal load was applied to the bottom surface of the model by imposing a fixed temperature of 100 °C, while the remaining surfaces were considered adiabatic. This configuration allowed the observation of one-dimensional heat flow without interference from convective or radiative effects, which were intentionally excluded to focus solely on conductive mechanisms.

Transient simulations were executed over a duration of 10 minutes, with thermal data extracted at time intervals of 1, 3, 5, and 10 minutes. A structured mesh was employed for both models, with higher node density near the heat source to capture steep thermal gradients. Mesh convergence testing was performed to ensure numerical stability and independence of results from mesh resolution.

Post-processing of simulation data included the extraction of temperature contours and thermal flux distributions at each time interval. These outputs enabled detailed observation of heat propagation dynamics and thermal gradient evolution within the two geometries. The microstructural BCC model was particularly instrumental in identifying anisotropic heat transfer pathways and delayed temperature equalization, providing insights into the role of microstructure in limiting the thermal conductivity in Ti6Al4V.

3. Results and Discussion

The CFD simulations conducted on Ti6Al4V under conduction-dominated conditions reveal distinct transient thermal behavior at both macro and microstructural scales. In the macroscopic simulation, where heat was applied uniformly to the bottom surface of a solid block, temperature evolution over a 10-minute period showed a delayed and highly non-uniform thermal response. As illustrated in Figure 1, the highest temperatures remained concentrated near the heat source, while the upper surface exhibited only modest increases. This confirms the limited thermal conductivity of Ti6Al4V, which inhibits efficient heat transfer along the vertical axis.

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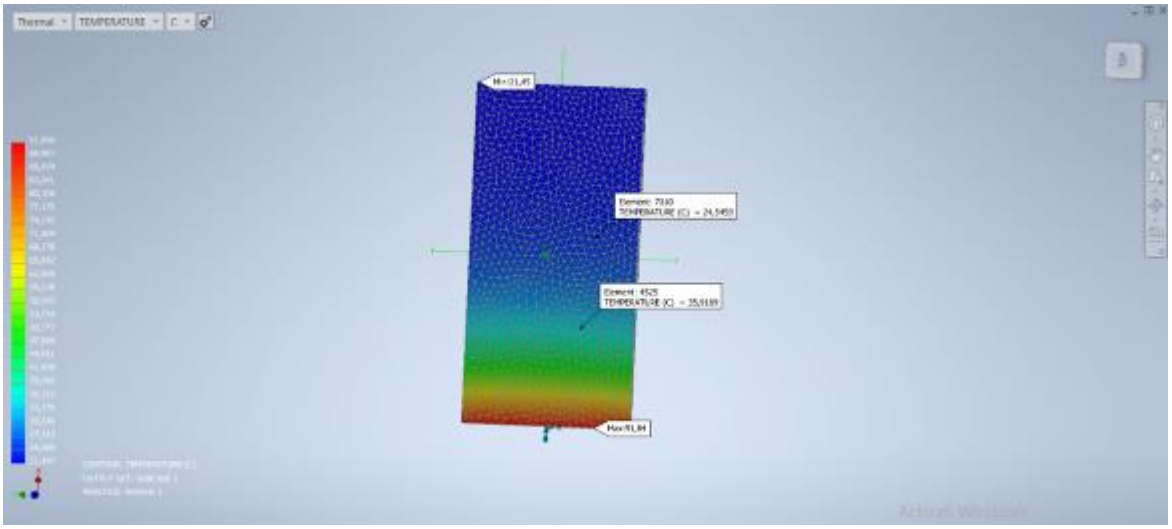

Fig. 1. *Simulated temperature field in a macroscopic Ti6Al4V block after 10 minutes of conduction-driven heating*

To better understand heat diffusion within the β-phase, a body-centered cubic (BCC) lattice model was employed (Figure 2). The simplified structure enabled the capture of directional conduction through the microstructure. Temperature snapshots taken at 1, 3, 5, and 10 minutes (Figures 3-6) show progressive, yet delayed, thermal diffusion from the base upward. At 1 minute, the temperature remained highly localized at the base, with minimal change in the upper lattice region. As heating continued, thermal propagation advanced slowly, becoming more uniform at 5 and 10 minutes, though vertical gradients persisted.

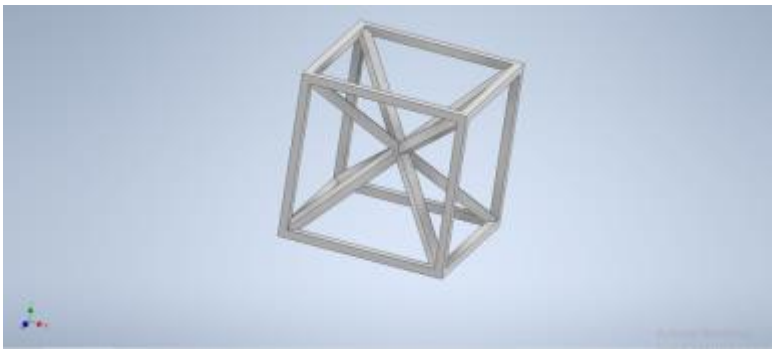

Fig. 2. *CAD-based geometric representation of a BCC lattice unit used to model the β-phase in Ti6Al4V*

These results reflect the alloy's intrinsic thermal resistance, governed by its low thermal diffusivity. Ti6Al4V yields a thermal diffusivity of 4.47×10^{-6} m^2/s, calculated via $\alpha = k / (\rho \cdot c_p)$.

This low α value supports the simulation findings of slow heat penetration and persistent temperature gradients.

In practical applications, these findings underscore the importance of accounting for Ti6Al4V's slow heat conduction, particularly in designs involving passive thermal management or transient thermal loads. While the material's mechanical and corrosion-resistant properties remain advantageous, its thermal limitations may necessitate the use of auxiliary cooling methods or hybrid material solutions in temperature-sensitive components. The CFD-based methodology used in this study has proven effective in isolating and analysing these material-specific thermal behaviours, offering a predictive framework for optimizing Ti6Al4V in thermally constrained environments.

This crystallographic arrangement contributes to the alloy's thermal behavior. The tightly packed atomic structure and directional bonding influence heat transfer, supporting the observed anisotropy in thermal distribution during simulation.

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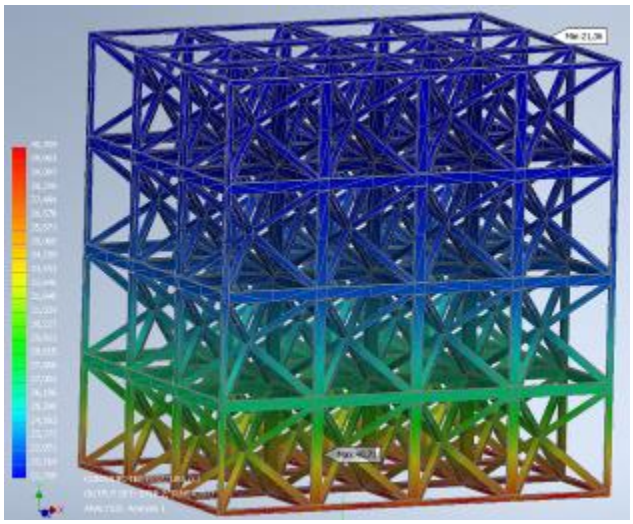

Fig. 3. *Simulated initial thermal propagation in the BCC lattice model of Ti6Al4V at t = 1 minute*

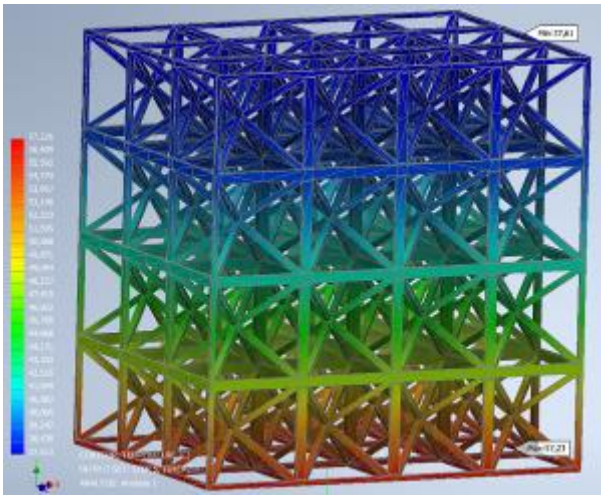

Fig. 4. *Simulated intermediate thermal propagation in the BCC lattice model of Ti6Al4V at t = 3 minutes*

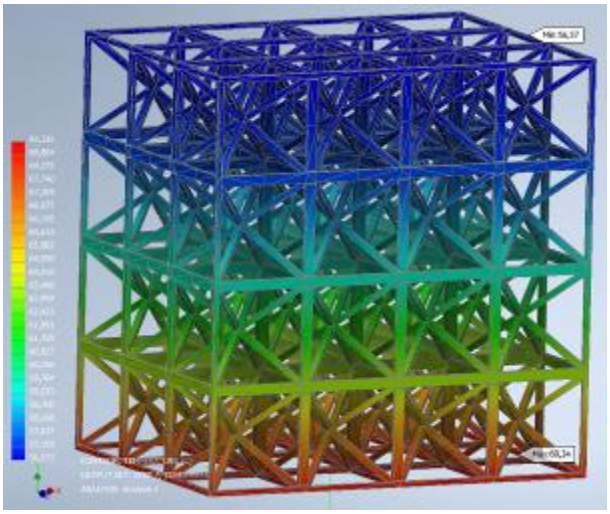

Fig. 5. *Simulated advanced thermal propagation in the BCC lattice model of Ti6Al4V at t = 5 minutes*

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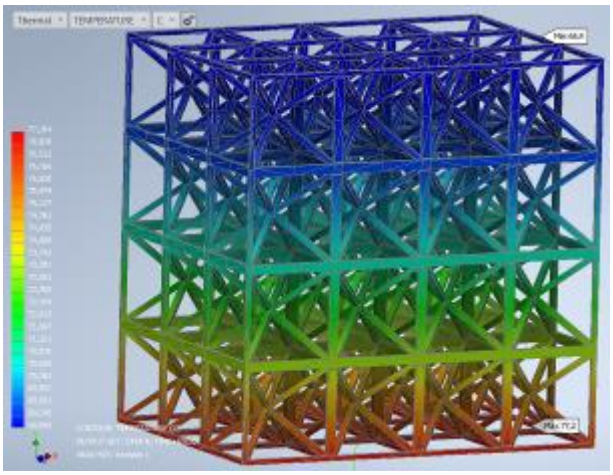

Fig. 6. *Quasi-steady-state thermal distribution in the BCC lattice model of Ti6Al4V at t = 10 minutes*

The thermal resistance observed in both simulations reflects the material's intrinsic properties. Based on the thermal diffusivity relation $\alpha = k / (\rho \cdot c_p)$, and using values of 6.5 W/m·K for conductivity, 4410 kg/m^3 for density, and 326 J/kg·K for specific heat, Ti6Al4V exhibits low α. This theoretical result aligns with the delayed thermal response in both the bulk and lattice domains. At the end of the simulation period (t = 10 min), the temperature at the base reached approximately 240 °C, while the top surface remained below 137 °C. This temperature gradient reinforces the slow thermal response and poor vertical conduction efficiency of Ti6Al4V.

The combined findings reinforce the conclusion that Ti6Al4V - although mechanically robust and corrosion resistant - is limited in its ability to quickly or uniformly dissipate heat. The thermal gradients persist well into the simulation period, indicating that the alloy is more suitable for applications where structural integrity is critical, but passive thermal management must be supplemented or reconsidered. CFD has proven to be a reliable tool in capturing both macroscopic heat flow and localized anisotropic behavior, providing a predictive framework for optimizing Ti6Al4V in thermally constrained environments.

4. Conclusions

This paper employed computational fluid dynamics (CFD) simulations to investigate the transient thermal behavior of the titanium alloy Ti6Al4V under conduction-dominated conditions. By combining macro-scale and microstructural models, the simulations provided valuable insights into both bulk and directional heat transfer characteristics of the material. The results consistently demonstrated a slow and non-uniform thermal response, with significant vertical gradients persisting throughout the simulation period. This behavior was evident in both the solid block and the BCC lattice models, indicating that the alloy's low thermal conductivity and thermal diffusivity fundamentally limit its ability to rapidly dissipate heat.

The microstructural simulations highlighted the influence of lattice structure on thermal propagation, particularly within the β-phase of Ti6Al4V. The BCC geometry revealed delayed and anisotropic heat conduction, with thermal gradients diminishing only gradually over time. These findings underscore the material's limitations in applications that require efficient and rapid thermal equalization, such as those involving cyclic thermal loading, high-power electronics, or additive manufacturing processes where thermal control is important to part integrity.

Despite these thermal constraints, Ti6Al4V remains a highly valuable material due to its exceptional mechanical properties, corrosion resistance, and biocompatibility. However, its use in thermally sensitive designs must be carefully considered. These findings suggest that while Ti6Al4V is structurally ideal, its thermal constraints demand strategic adaptations in design when used in temperature-sensitive environments.

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