**Introduction:**

Since the 20th century Titanium (Ti) alloys have commonly been a key part in aircraft design due to their incredible strength-to-weight ratio, intrinsic corrosion resistance, and high melting point. Since then, Ti alloys have expanded to become a critical material in biomedical and automotive industries, making it a special interest to researchers. Commercially pure (C.P.) titanium alloys exhibit two phases at low pressures, with a transition temperature of approximately 882°C [1]. The α-Ti phase, stable at lower temperatures, has a hexagonal close-packed (hcp) crystal structure, while the β-Ti phase, which is stable at higher temperatures, adopts a body-centered cubic (bcc) structure.

During heat treatment Ti experiences an increase in grain size. Understanding the microstructure, and therefore the mechanical properties, of Ti alloys is important when understanding how it can be used. This phenomenon has been described by the Hall-Petch relationship [2] which notes the inverse relationship between grain size and yield strength. As grains grow, the barriers to dislocation movement are reduced as the number of grain boundaries decrease, impacting the strength of the material. To optimize mechanical properties this phenomenon in Ti must be studied. However, experimental grain growth research for Ti alloys is limited. Here, isothermal grain growth simulations are created using the Phase Field Method (PFM) above and below the transition temperature to explore temperature dependent trends across phases. Simulation results are compared to experimental data to ensure model accuracy for future advancements.

**Methodology:**

PFM represents the microstructure of a material using conserved and nonconserved field variables that represent the evolution of physical properties and the microstructure of the material, respectively. For grain growth, the Allen-Cahn equation describes the evolution of the nonconserved order parameters as , where *F* is the free energy functional, *L* is the order parameter mobility, and is the order parameter variation [3]. Hence, the free energy functional is defined as , where *k* and *L* are described in terms of the model parameters.

The model parameters consist of the grain mobility prefactor (), activation energy (*Q*), and grain boundary energy (). These parameters are extrapolated from experimental data [4-7], with specifically determined using the Arrhenius equation: . Due to a gap in the literature, M values were determined using the Burke-Turnbull equation [8].

The grain growth rate is defined using the exponent *n* in , where K is a material constant and ​, are the final and initial grain diameters, respectively. When is very small, it can be ignored, simplifying the determination of *n* using [9]. Activation energy for atomic diffusion across grain boundaries is crucial for describing growth, with α-Ti exhibiting a higher activation energy due to its greater packing efficiency in the hcp structure compared to bcc in β-Ti.

**Discussion of Results:**

Simulated growth output closely matches experimental results. However, experimentally, growth occurs at a higher rate for β-Ti and reports higher growth exponent values on average. However, relying on experimental values for the input parameters yields the opposite result in this model, where β-Ti experiences a lower growth rate on average. This may be attributed to the temperatures at which single-phase growth is measured, as β-Ti exists at higher temperatures resulting in a higher growth exponent. While growth occurs more readily in β-Ti, α-Ti’s favorable input parameters leads to rapid growth once thermodynamically favorable. While literature regarding single-phase interface mobility is scarce for Ti, a sensitivity analysis must be done using stochastic tools to explore the input parameter’s relative effect on the growth exponent. Finally, work has been done to mimic the effects of irradiation on isothermal grain growth with an additional Allen-Cahn-like term to the free energy functional [10]. To model ion-induced grain growth this term can be introduced by adding “thermal spikes” at or around grain boundaries. These spikes induce atomic diffusion by increasing the temperature by approximately 1000K, lasting approximately 10-11 seconds.

**References:**

[1] Jafari, M., Vaezzadeh, M. & Noroozizadeh, S. Thermal Stability of *α* Phase of Titanium by Using X-Ray Diffraction. *Metall Mater Trans A* 41, 3287–3290 (2010). <https://doi.org/10.1007/s11661-010-0393-1>

[2] Z.W. Huang, P.L. Yong, H. Zhou, Y.S. Li, Grain size effect on deformation mechanisms and mechanical properties of titanium, Materials Science and Engineering: A, Volume 773, 2020, 138721, ISSN 0921-5093, https://doi.org/10.1016/j.msea.2019.138721.

[3] Long-Qing Chen, A novel computer simulation technique for modeling grain growth, Scripta Metallurgica et Materialia, Volume 32, Issue 1, 1995, Pages 115-120, ISSN 0956-716X, https://doi.org/10.1016/S0956-716X(99)80022-3.

[4] Héléna Verbeeck, Vincent Feyen, Pushkar Prakash Dhekne, Nele Moelans, Scale-bridging phase-field approach for nucleation and microstructure evolution applied to the β to α phase transformation in pure titanium, Materials & Design, Volume 239, 2024, 112768, ISSN 0264-1275, <https://doi.org/10.1016/j.matdes.2024.112768>.

[5] Najafkhani, F., Kheiri, S., Pourbahari, B. *et al.* Recent advances in the kinetics of normal/abnormal grain growth: a review. *Archiv.Civ.Mech.Eng* 21, 29 (2021). <https://doi.org/10.1007/s43452-021-00185-8>

[6] Wang, H., Bao, Q.L., Zhou, G. *et al.* Dynamic recrystallization initiated by direct grain reorientation at high-angle grain boundary in α-titanium. *Journal of Materials Research* 34, 1608–1621 (2019). <https://doi.org/10.1557/jmr.2019.125>

[7] Di Qiu, Pengyang Zhao, Chen Shen, Weijie Lu, Di Zhang, Matous Mrovec, Yunzhi Wang, Predicting grain boundary structure and energy in BCC metals by integrated atomistic and phase-field modeling, Acta Materialia, Volume 164, 2019, Pages 799-809, ISSN 1359-6454, <https://doi.org/10.1016/j.actamat.2018.11.023>.

[8] J. Burke, D. Turnbull, Recrystallization and grain growth, Prog. Met. Phys. 3 (1952) 220–292, https://doi.org/10.1016/0502-8205(52)90009-9.

[9] Xu Y, Tang D, Song Y, Pan X. Prediction model for the austenite grain growth in a hot rolled dual phase steel. Mater Des. 2012;36:275–8

[10] ] D.E. Alexander, G.S. Was, Thermal-spike treatment of ion-induced grain growth: Theory and experimental comparison, Phys. Rev. B 47 (1993) 2983–2994.