CP301 – DEVELOPMENT ENGINEERING PROJECT

HEMIs GV – STUDIO

Acronym ‘HEMIs GV’

‘Hypersonic Environment for missiles and Glide Vehicles’

Under the supervision of,

Dr. Pratik K. Ray

Department of Metallurgical and Materials Engineering

Indian Institute of Technology, Ropar

Submitted by,

HIMANSHU PARGANIHA – 2020MMB1346

VAIBHAVI SANJIVKUMAR PATIL – 2020MMB1359

❖ INTRODUCTION

Why the study of Hypersonics?

Hypersonics is a field of study that involves the study of vehicles that travel at extremely high speeds, typically above Mach 5 or five times the speed of sound. The field of hypersonics is of great interest because of the numerous potential applications in military, scientific, and commercial fields.

The study of hypersonics is important because it allows us to design and develop vehicles that can travel at extremely high speeds, enabling us to explore and study the upper atmosphere and space, develop new military technologies and capabilities, and design commercial transport vehicles that are faster and more efficient. Additionally, the study of hypersonics involves many challenging and complex scientific and engineering problems, making it a fascinating field of research that continues to attract scientists and engineers from around the world.

Substantial Oxidation Behaviour

Oxidation is a significant factor in the field of hypersonics due to the extreme temperatures and velocities experienced by vehicles in hypersonic flight. Oxidation can cause material degradation and failure, which can have catastrophic consequences for the vehicle and its occupants. Therefore, understanding and predicting oxidation behaviour is crucial for the successful design and operation of hypersonic vehicles.

- Ways in which oxidation can influence hypersonic flight:

1. Oxidation can cause erosion, corrosion, and other forms of damage to the surfaces of hypersonic vehicles, affecting their aerodynamics and thermal protection.
2. Oxidation can increase the weight of the vehicle due to the formation of oxides, which can affect its performance and manoeuvrability.
3. The oxidation process can generate heat, which can further exacerbate the already extreme thermal environment of hypersonic flight.
4. The reaction between the metal and the oxidizer can produce gases, which can affect the vehicle's stability and manoeuvrability.

5. The rate of oxidation can depend on various factors such as temperature, pressure, and the composition of the material, making it a complex phenomenon to model and predict accurately.

Brief Overview of the Model

Simulating the oxidation behaviour of Haynes 282 alloy at high temperatures. In this model, the microstructure of the alloy is divided into a grid of cells, and the oxidation of each cell is modelled individually using rules based on the diffusion of oxygen and other species, as well as the Gibbs free energy of the oxidation reactions.

The model calculates the oxidation rate of each cell using the formula

$$V = A * J * N_A * M$$

Where,

A is the surface area of the cell

J is the diffusion flux

N_A is Avogadro's number

M is the molar mass of the metal

The diffusion flux is calculated using Fick's laws of diffusion, and the Gibbs free energy is calculated using thermodynamic data for the various oxides that may form during oxidation.

The output of the model is a grid pattern showing the progression of oxidation over time at a specific temperature, which can be used to predict the oxidation behaviour of the alloy and inform material design and engineering decisions.

❖ LITERATURE REVIEW

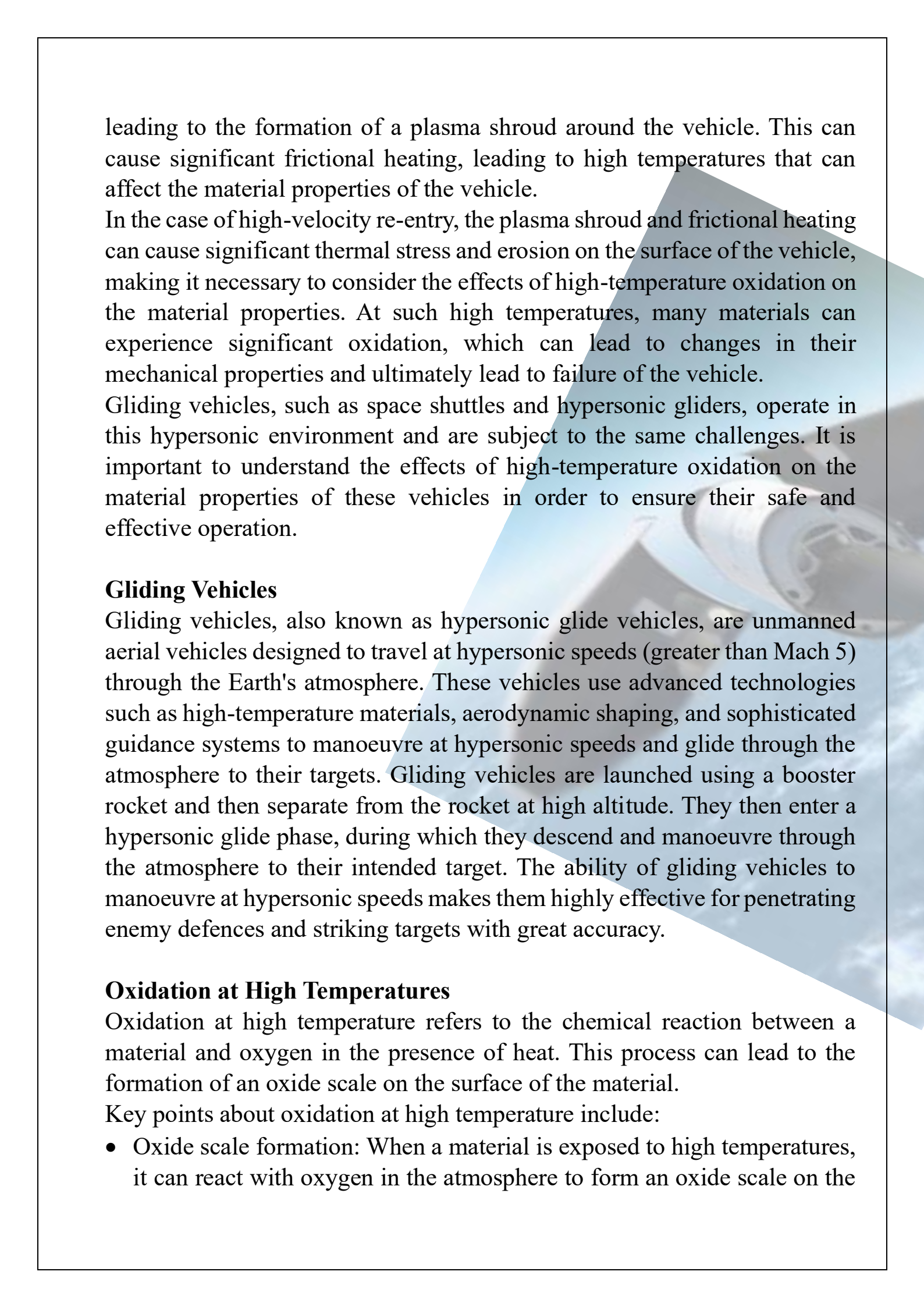
Hypersonic Environment

Hypersonic environment refers to the conditions experienced by objects traveling at hypersonic speeds, which is typically defined as speeds exceeding Mach 5 (i.e., five times the speed of sound). At such velocities, the air around an object in flight becomes highly compressed and heats up,

leading to the formation of a plasma shroud around the vehicle. This can cause significant frictional heating, leading to high temperatures that can affect the material properties of the vehicle.

In the case of high-velocity re-entry, the plasma shroud and frictional heating can cause significant thermal stress and erosion on the surface of the vehicle, making it necessary to consider the effects of high-temperature oxidation on the material properties. At such high temperatures, many materials can experience significant oxidation, which can lead to changes in their mechanical properties and ultimately lead to failure of the vehicle.

Gliding vehicles, such as space shuttles and hypersonic gliders, operate in this hypersonic environment and are subject to the same challenges. It is important to understand the effects of high-temperature oxidation on the material properties of these vehicles in order to ensure their safe and effective operation.



Gliding Vehicles

Gliding vehicles, also known as hypersonic glide vehicles, are unmanned aerial vehicles designed to travel at hypersonic speeds (greater than Mach 5) through the Earth's atmosphere. These vehicles use advanced technologies such as high-temperature materials, aerodynamic shaping, and sophisticated guidance systems to manoeuvre at hypersonic speeds and glide through the atmosphere to their targets. Gliding vehicles are launched using a booster rocket and then separate from the rocket at high altitude. They then enter a hypersonic glide phase, during which they descend and manoeuvre through the atmosphere to their intended target. The ability of gliding vehicles to manoeuvre at hypersonic speeds makes them highly effective for penetrating enemy defences and striking targets with great accuracy.

Oxidation at High Temperatures

Oxidation at high temperature refers to the chemical reaction between a material and oxygen in the presence of heat. This process can lead to the formation of an oxide scale on the surface of the material.

Key points about oxidation at high temperature include:

- Oxide scale formation: When a material is exposed to high temperatures, it can react with oxygen in the atmosphere to form an oxide scale on the

surface. This oxide scale can act as a protective layer, slowing down further oxidation and protecting the underlying material from further damage.

- Mechanism: The mechanism of oxide scale formation depends on several factors, including the type of material being oxidized, the temperature and pressure of the environment, and the presence of other chemical species. Generally, the process involves the diffusion of oxygen through the oxide layer and the reaction of the oxygen with the underlying material.
- Factors affecting and dependence: The rate of oxidation depends on a number of factors, including the temperature, the oxygen partial pressure, the composition of the material being oxidized, and the nature of any protective coatings or oxide layers. High temperatures and high oxygen partial pressures can increase the rate of oxidation, while protective coatings or oxide layers can slow it down.
- Threats to the component/material: Oxidation at high temperatures can lead to a number of threats to the component or material being oxidized. These include reduced mechanical properties, such as strength and ductility, and reduced resistance to fatigue and fracture. In extreme cases, oxidation can lead to component failure and catastrophic loss.

Super Alloys Vs. High Temperature Ceramics

	Superalloys	**High Temperature Ceramics**
Composition	Mainly metallic alloys	Non-metallic compounds
Strength	High strength at high temperatures	Generally lower strength than superalloys
Toughness	Generally high toughness and ductility	Brittle behaviour
Oxidation	Can form protective oxide scales	Typically, do not form protective oxide scales
Thermal	High thermal conductivity and expansion	Low thermal conductivity and expansion
Stability	Generally stable at high temperatures and loads	Susceptible to thermal shock and mechanical loads
Applications	Turbine blades, exhaust systems, heat exchangers	Insulators, thermal barriers, rocket nozzles

NI – Based Superalloys

1. Ni-based superalloys are high-performance materials that are specifically designed to withstand extreme environments, such as high temperatures and corrosive atmospheres.
2. They are composed of a mixture of nickel, cobalt, iron, and other alloying elements, such as chromium, aluminium, and titanium, that provide high-temperature strength, corrosion resistance, and oxidation resistance.
3. The microstructure of Ni-based superalloys is characterized by a fine-grained matrix that is reinforced by a network of fine, coherent, and semi-coherent precipitates that provide additional strength and stability.
4. Ni-based superalloys are commonly used in gas turbine engines for aerospace, power generation, and other high-performance applications where high-temperature strength, corrosion resistance, and thermal stability are critical.
5. They have excellent creep and fatigue resistance, good weldability and formability, and can maintain their properties even at temperatures up to 1200°C.
6. The development of Ni-based superalloys is a continuous process, with researchers and engineers constantly exploring new alloy compositions, processing techniques, and microstructural design strategies to enhance their performance and reliability.

HAYNES 282

Why Haynes 282, its features, and applications →

Haynes-282 is a nickel-based superalloy developed by Haynes International, Inc. It is designed to have exceptional resistance to high-temperature corrosion and oxidation, making it an ideal material for use in high-temperature applications.

FEATURES→

- High-temperature strength: Haynes 282 is able to maintain its strength even at temperatures as high as 982°C (1800°F). This makes it well-suited for use in applications where high-temperature strength is critical.

- Corrosion resistance: The alloy has excellent resistance to high-temperature corrosion and oxidation, particularly in environments containing sulphur. This makes it suitable for use in harsh industrial environments.
- Weldability: Haynes 282 is relatively easy to weld, making it an attractive option for applications that require the use of welded joints.

APPLICATIONS→

- Turbine blades and vanes: Haynes 282 is used in the manufacture of turbine blades and vanes for aircraft engines, due to its excellent resistance to high-temperature corrosion and oxidation. The alloy is known to maintain its strength and corrosion resistance even at temperatures exceeding 1000°C, making it ideal for use in jet engines.
- Afterburner components: The alloy's ability to withstand high temperatures and maintain strength and corrosion resistance make it a suitable material for use in afterburner components in jet engines. These components require materials that can withstand high temperatures and high-stress environments.
- Heat exchangers: Haynes 282 is used in the manufacture of heat exchangers for aircraft engines, due to its high-temperature stability and excellent resistance to oxidation and corrosion. Heat exchangers are used to transfer heat between fluids and are an essential component in many aerospace applications.

❖ STUDY OF NI-BASED SUPERALLOY – HAYNES 282

COMPOSITION: (in wt%)

Ni	Cr	Co	Mo	Ti	Al	Fe	Mn	Si	C	B
55.23	19	10	9.5	2.55	1.7	1.5	0.3	0.15	0.060	0.005

OXIDES DIFFUSION COEFFICIENT:

Cr_2O3	TiO_2	Al_2O_3
$10^{-11}m^2/s$	$10^{-12}m^2/s$	$10^{-11}m^2/s$

HIGH TEMPERATURE CHARECTERISTICS:

- Protective oxide scale formation: When exposed to high-temperature oxidizing environments, Haynes 282 forms a protective oxide scale consisting of mainly Cr2O3, Al2O3, and NiO.
- Oxidation resistance at high temperatures: Haynes 282 exhibits excellent oxidation resistance up to 1000°C, with only a slight increase in the oxidation rate above this temperature.

HIGH TEMPERATURE BEHAVIOUR:

Alloy's constituent elements: nickel, cobalt, chromium, and aluminium, with oxygen in the air.
This reaction leads to the formation of metal oxides, such as NiO, CoO, Cr2O3, and Al2O3, on the surface of the alloy.

1. The oxidation of nickel:
   $2Ni + O_2 \rightarrow 2NiO$
2. The oxidation of cobalt:
   $2Co + O_2 \rightarrow 2CoO$
3. The oxidation of chromium:
   $4Cr + 3O_2 \rightarrow 2Cr_2O_3$
4. The oxidation of aluminium:
   $4Al + 3O_2 \rightarrow 2Al_2O_3$
5. Formation of complex oxides, such as spinels:
   $(Al, Co, Ni)_2O_4 + Cr_2O_3 \rightarrow (Al, Co, Ni, Cr)_2O_4$

ORDER OF OXIDE FORMATION:

1. Aluminium oxide (Al2O3) - forms first on the surface of the alloy due to the high affinity of aluminium for oxygen.
2. Cobalt oxide (CoO) and nickel oxide (NiO)
3. Chromium oxide (Cr2O3) - forms at a slightly higher temperature than cobalt and nickel oxides
4. Spinel (Al, Co, Ni, Cr)2O4 - forms when the above oxides react with Cr2O3 to form the stable and protective spinel layer on the surface of the alloy.

❖ MATHEMATICS

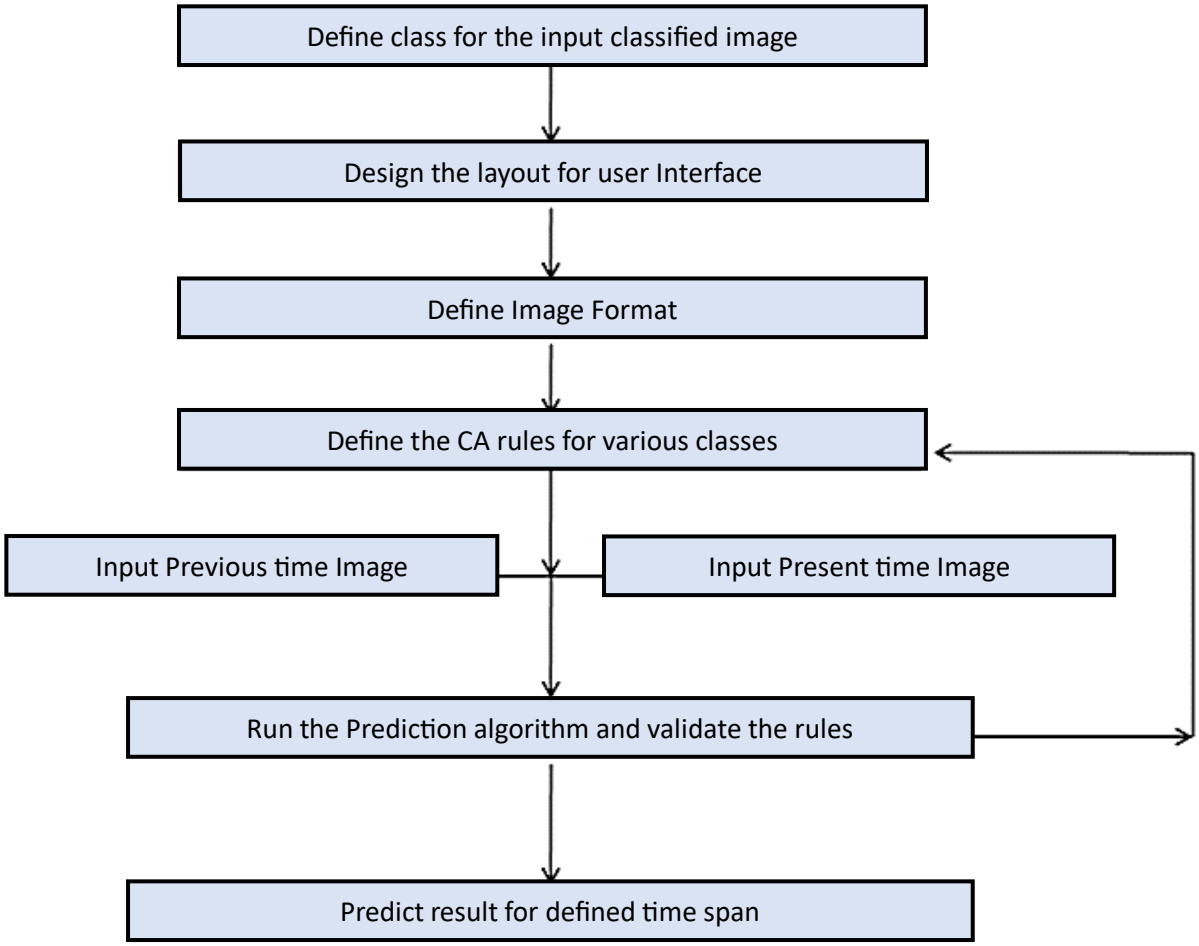
Cellular Automata Model

Cellular automata (CA) is a model that simulates complex systems using a grid of cells with a set of rules governing the behaviour of each cell.
CA models can be either deterministic, meaning that the rules governing the state of each cell are fixed and predictable, or stochastic, meaning that there is some randomness in the rules.

Feature	Deterministic CA	Stochastic CA
Update rule	Same rule applied to all cells	Random rule applied to each cell
State transition	Deterministic	Probabilistic
State at next time step	Computed exactly	Randomly determined
Initial state	Determines entire evolution	Determines initial probabilities for evolution
Behaviour	Predictable	Non-deterministic
Examples	Game of Life	Forest fire simulation

Brief overview of the steps involved in a typical CA model:

1. Define the grid size: Decide the dimensions of the grid (the number of rows and columns).
2. Define the initial state of the grid: Determine the initial state of each cell in the grid. This could be random or predetermined.
3. Define the rules: Determine the set of rules that govern the behaviour of each cell. The rules could be simple or complex, and can be based on various factors such as the state of neighbouring cells or time.
4. Apply the rules: Apply the rules to each cell to determine its new state.
5. Repeat: Repeat steps 3 and 4 for each time step until the desired simulation duration is reached.
6. Visualize the results: Visualize the state of the grid at each time step using a graphical representation such as an image or animation.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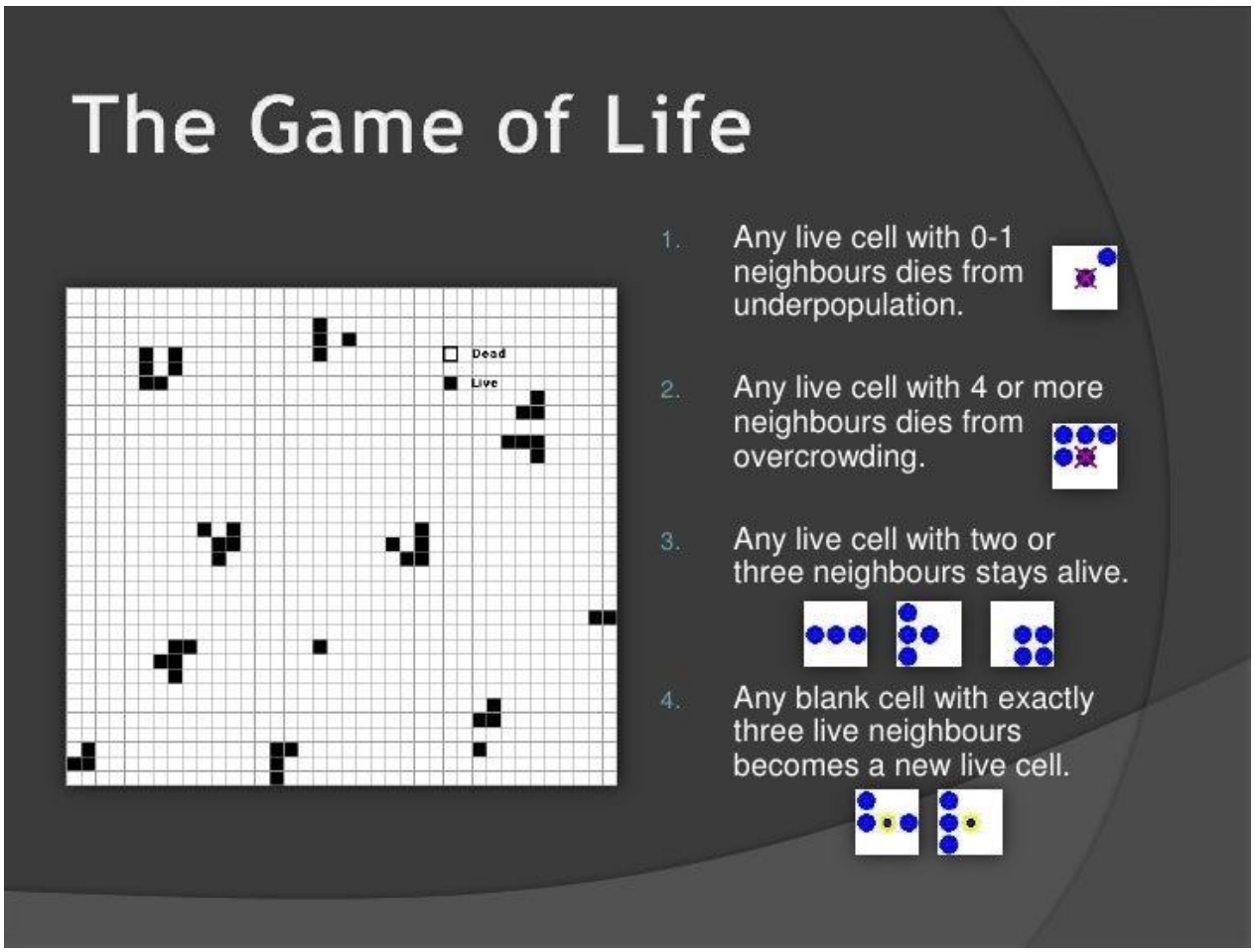
Design the layout for user Interface
Define Image Format
Define the CA rules for various classes
Input Previous time Image
Input Present time Image
Run the Prediction algorithm and validate the rules
Predict result for defined time span


The Game of Life
Dead
Live
1. Any live cell with 0-1 neighbours dies from underpopulation.
2. Any live cell with 4 or more neighbours dies from overcrowding.
3. Any live cell with two or three neighbours stays alive.
4. Any blank cell with exactly three live neighbours becomes a new live cell.

Study of Related Mathematical Frameworks

A. MONTE CARLO METHOD

The Monte Carlo method is a stochastic simulation method used to model complex systems that involve probabilistic behaviour. It is based on generating random numbers and using them to simulate the system behaviour. In mathematical terms, it involves computing an expectation value of a function of interest by generating random samples from the probability distribution of the system. The method can be used to solve a variety of problems in physics, engineering, and other fields, and is particularly useful when the system is too complex to be modelled analytically.

B. Q-STATE POTTS MODEL

The Q-state Potts model is a mathematical model used to study the behaviour of systems with multiple states. It is based on a lattice of spins, where each spin can take on one of Q discrete values. The model is used to study the phase transitions that occur in these systems, such as the transition from a disordered state to an ordered state as the temperature is lowered. The Hamiltonian of the model is given by a sum over pairs of neighbouring spins, and the partition function is computed using a sum over all possible spin configurations.

C. MARKOV CHAIN MODEL

The Markov chain model is a stochastic model used to describe the evolution of a system over time. It is based on a set of states and transition probabilities between those states. The model assumes that the probability of moving from one state to another depends only on the current state and not on any previous states. The model can be used to analyse a wide range of systems, such as population dynamics, financial markets, and genetic algorithms. The mathematics behind the model involve computing the stationary distribution of the system, which is the long-term distribution of states that the system tends towards as time goes to infinity.

Correlation with the case study of Haynes 282

Monte Carlo method:

- ➔ Used to simulate the diffusion of oxygen atoms in the alloy by randomly selecting oxygen atoms and allowing them to diffuse through the lattice structure of the alloy.
- ➔ The probability of diffusion is determined by the local concentration of oxygen atoms and the temperature of the system.
- ➔ By repeating this process many times, the Monte Carlo method generates a statistical distribution of oxygen atom diffusion, which is used to predict the overall rate of oxidation.

Q-state Potts model:

- ➔ Used to simulate the formation of oxide scales on the surface of the alloy by assigning different "spin states" to each lattice site, which represent the different oxidation states of the alloy.
- ➔ The probability of transitioning from one spin state to another is determined by the local concentration of oxygen atoms and the temperature of the system.
- ➔ By repeating this process many times, the Q-state Potts model generates a statistical distribution of oxide scale formation, which is used to predict the morphology and thickness of the oxide scale.

Markov chain model:

- ➔ Used to simulate the evolution of the oxide scale over time by representing the oxide scale as a set of discrete states, where each state corresponds to a different morphology or thickness of the oxide scale.
- ➔ The probability of transitioning from one state to another is determined by the local concentration of oxygen atoms and the temperature of the system.
- ➔ By repeating this process many times, the Markov chain model generates a statistical distribution of oxide scale evolution, which is used to predict the long-term behaviour of the oxide scale.

❖WORKING OF THE MODEL

Designing the Algorithm

A model to simulate the oxidation behaviour of Haynes 282 alloy in hypersonic environments based on the composition of the alloy and the diffusivity of the various compounds involved in the oxidation process.

DIFFUSIVITY:
The diffusivity of the various compounds involved in the oxidation process will also affect the rate of oxidation. The diffusivity of oxygen in the alloy and the diffusivity of the oxide compounds in the oxide layer can be calculated using **Fick's laws of diffusion**

STEPS-

1. Initialize the microstructure: Create a 2D grid of cells, where each cell represents a small area on the surface of the alloy. Assign an initial state to each cell, such as "metallic" to represent unoxidized material.
2. Set the simulation parameters: Define the temperature of the environment such as 1000 degree Celsius, and set the simulation time step and simulation duration.
3. Calculate the oxidation rate: For each cell in the grid, calculate the oxidation rate based on the local environment and properties of the cell.
4. Update the cell states: Based on the calculated oxidation rate, update the state of each cell to reflect its new oxidation state. For example, cells that were in the metallic state might now transition to the oxide state, and cells in the oxide state might thicken or thin depending on the oxidation rate.
5. Repeat the process: Continue calculating the oxidation rate and updating the cell states at each time step, until the simulation duration is reached.
6. Visualize the results: by plotting the grid pattern of the cell states at different time intervals. generate a grid pattern for every hour of simulation time, and plot these patterns in a series to show the progression of the oxidation behaviour over time.

Rules Driving the Oxidation

OXIDATION RATE CALCULATION –

In terms of diffusivity assuming a cuboid sample

I] Diffusion Coefficient

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

D^O – preexponential factor

(Extracted from experimental data)

II] Diffusion Flux

Fick's first law of diffusion

$J = -D \frac{\partial C}{\partial x}$

C – Concentration of oxidizing species

x – position

III] Volume of Cuboid = lbh

Surface Area = A (of one cell)

Rate of oxidation $\propto$ Diffusion Flux

Rate of oxidation (dm/dt) – mol s^{-1}

Oxidation Rate = A × J (mol s^{-1})

Oxidation rate in terms of mass of metal oxidized per unit time →

Oxidation Rate = A × J × N_A × M

M – Molar mass

A – Surface Area of one cell

J – Diffusion Flux

N_A – Avogadro's Number (6.022 * 10^{23} particle mol^{-1})

❖SIMULATION

Technical Requirements and stacks

- Python programming language: The code is written in Python, which is a high-level programming language known for its simplicity and ease of use. Python is widely used for scientific computing, data analysis, and machine learning applications.
- NumPy: NumPy is a Python library used for numerical computing. It provides powerful data structures for working with large arrays and matrices, along with a wide range of mathematical functions for performing various operations on these arrays.
- OpenCV: OpenCV is an open-source computer vision library that provides a wide range of tools and algorithms for image and video processing. In this model, OpenCV is used for reading and writing image and video files, as well as for resizing and converting images to grayscale.
- Matplotlib: Matplotlib is a Python library used for creating static, animated, and interactive visualizations in Python. In this model, Matplotlib is used for creating and saving visualizations of the simulated diffusion process.
- Scikit-image: scikit-image is a Python library used for image processing and computer vision applications. In this model, scikit-image is used for resizing and converting images to grayscale.
- PIL library: The Python Imaging Library (PIL) adds image processing capabilities to the Python interpreter. It is used in this model for resizing images.
- Jupyter Notebook: Jupyter Notebook is an open-source web application that allows users to create and share documents that contain live code, equations, visualizations, and narrative text. In this model, Jupyter Notebook is used as the development environment for writing and executing the code.
- Google Colab: Google Colab is a cloud-based Jupyter Notebook environment that provides free access to GPUs and TPUs for running

machine learning models. It is used in this model for running the code on a cloud-based machine.

Code and Simulation

(Trialled and not optimised version)

CODE SNIPPET

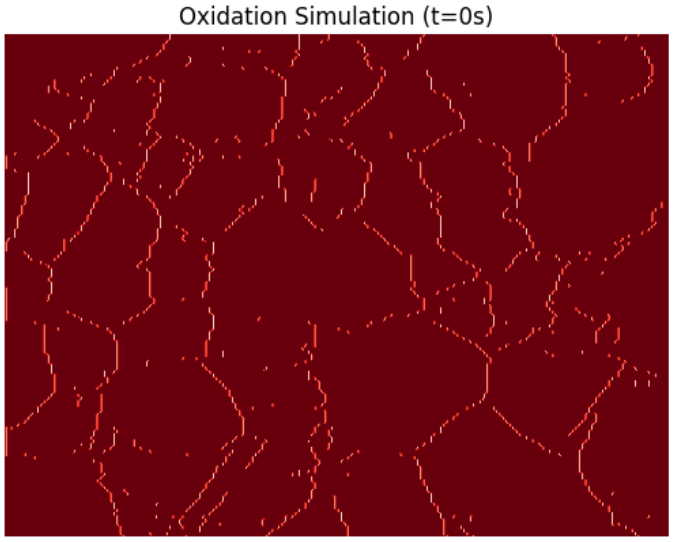
The oxidation simulation snippet:

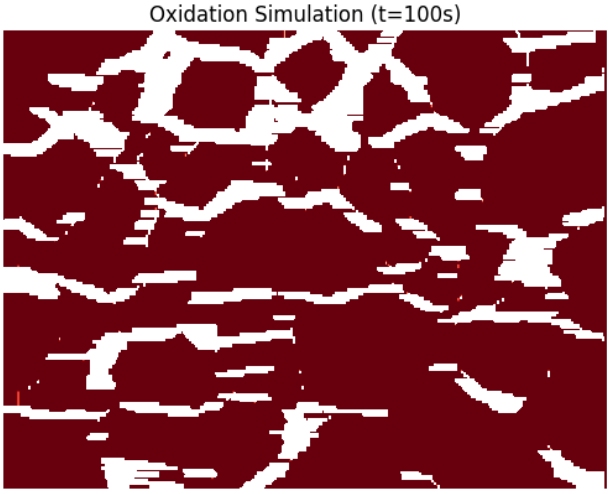
```
#OXIDATION SIMULATION
for t in range(0, duration, time_step):
    oxidation_rates = np.zeros(grid_size)              #Calculate oxidation rate for each cell in the grid
    for i in range(grid_size[0]):
        for j in range(grid_size[1]):
            C = 1                                      #(arbitrary value)
            oxidation_rates[i][j] = calculate_oxidation_rate(T, D0, Q, R, C, r, M)

    for i in range(grid_size[0]):                      #Update cell states based on calculated oxidation rate
        for j in range(grid_size[1]):
            if grid[i][j] == "metallic":
                if np.random.random() < oxidation_rates[i][j]:
                    grid[i][j] = "oxide"
            elif grid[i][j] == "oxide":
                thickness = 1 + oxidation_rates[i][j]  #Adjusting oxide thickness based on oxidation rate
                if np.random.random() < 0.5:
                    thickness *= -1
                new_thickness = max(0, min(thickness, 5))
                if new_thickness == 0:
                    grid[i][j] = "void"
                else:
                    grid[i][j] = "oxide" * new_thickness
```

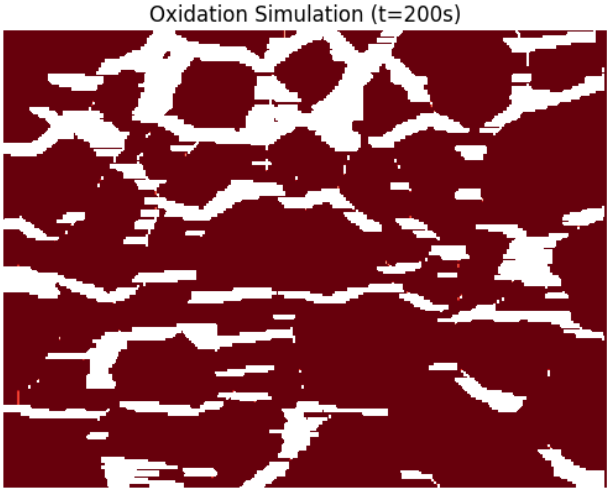
Image processing of Haynes 282 microstructure

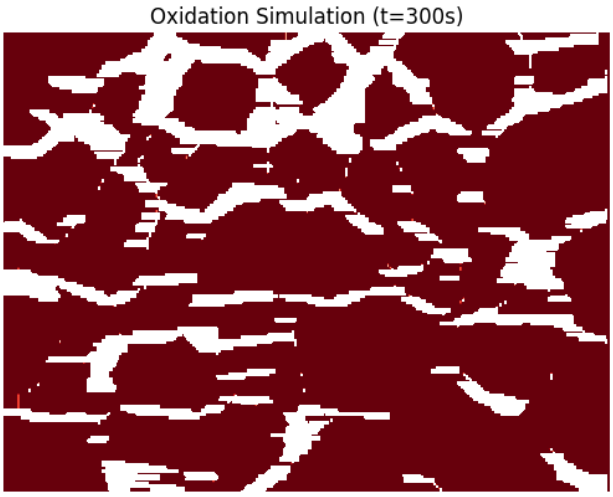
```
import cv2
import numpy as np

img = cv2.imread('Haynes03.png')              #Read the input image

gray = cv2.cvtColor(img, cv2.COLOR_BGR2GRAY) #Convert the image to grayscale

gray = cv2.medianBlur(gray, 3)                #Apply a median blur to remove noise

edges = cv2.Canny(gray, 50, 150)              #Apply a Canny edge detector to detect edges

kernel = np.ones((3,3), np.uint8)             #Dilate the edges to make them thicker
dilated_edges = cv2.dilate(edges, kernel, iterations=1)

inverted_edges = cv2.bitwise_not(dilated_edges)

result = cv2.bitwise_and(img, img, mask=inverted_edges)

cv2.imwrite('microstructure_edges.png', result)
```

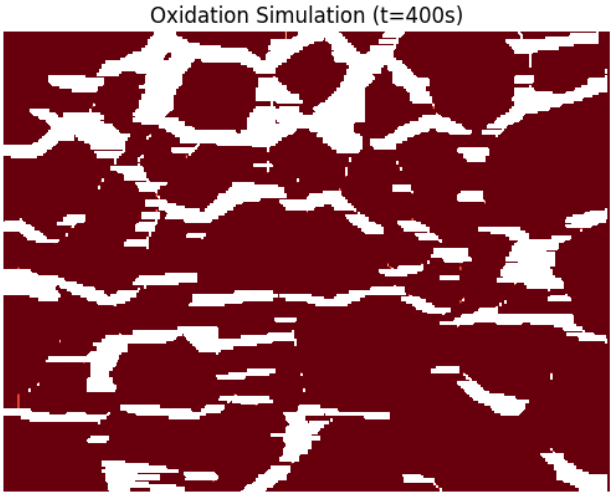
Simulation Output





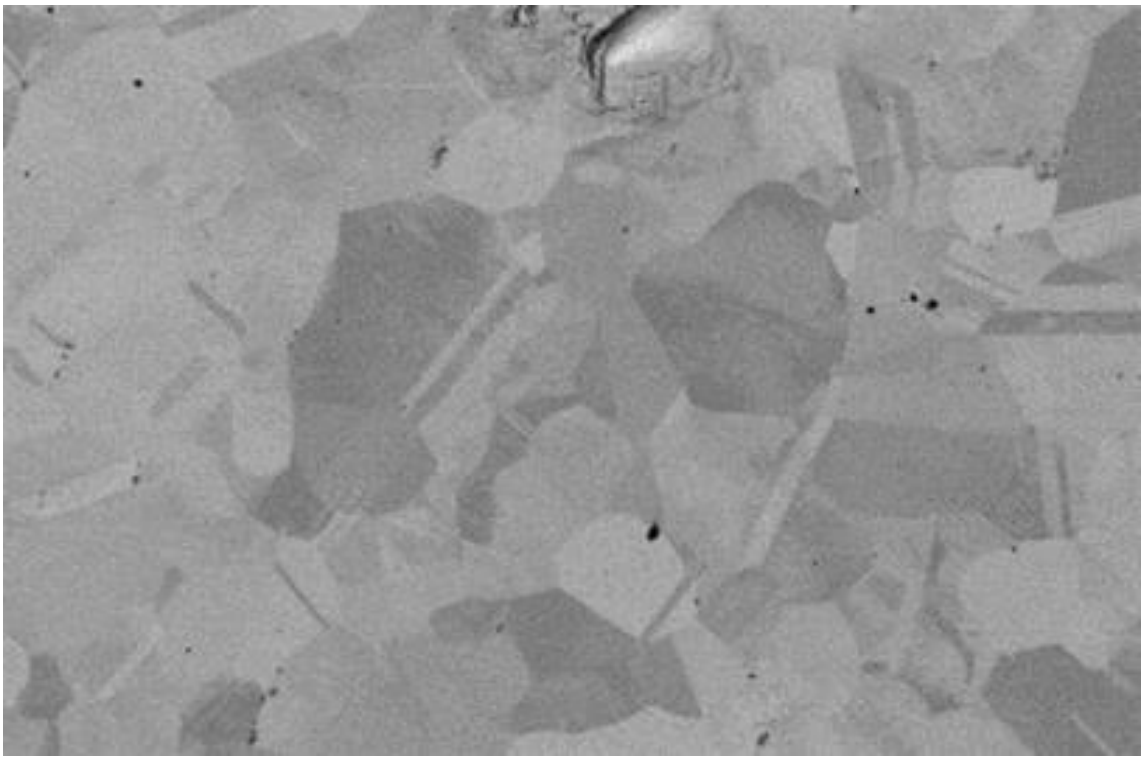


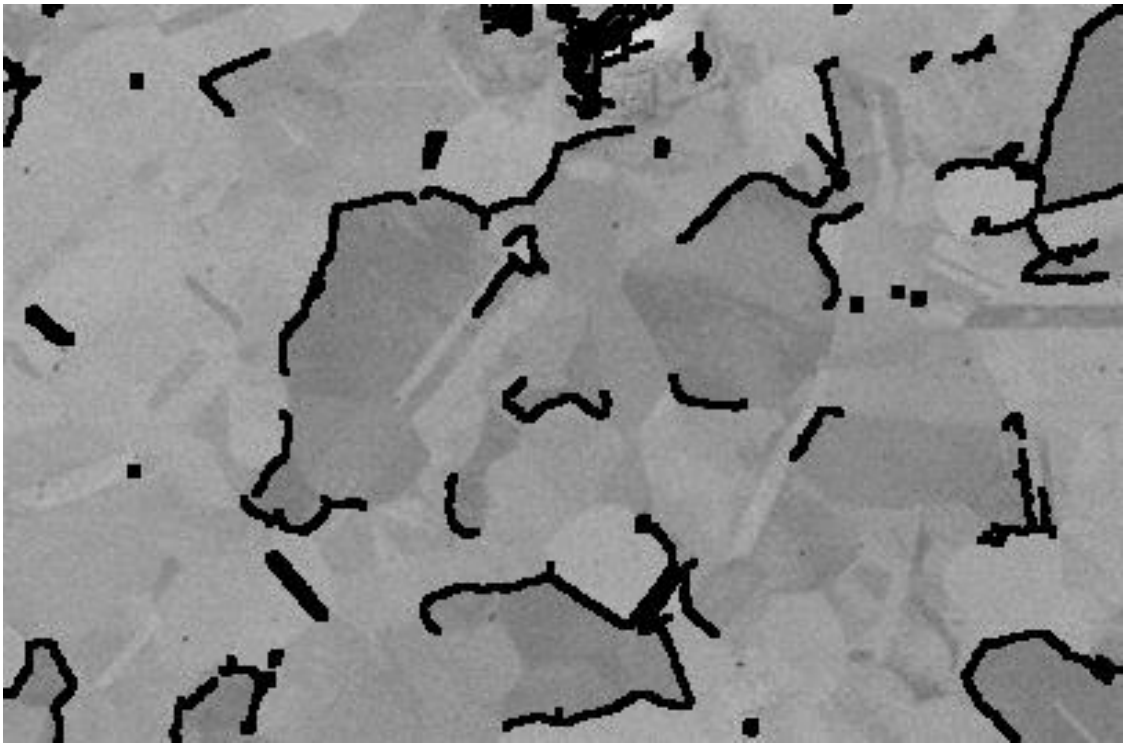




Till 1500sec

Image processing





❖ DISCUSSION

ANALYSIS OF THE OUTPUT

The simulation model needs to be run for a sufficient amount of time to capture the dynamics of the oxidation process accurately. In this case, since the model could not run for enough time, the images generated may not show the complete picture of the oxidation process. They may only capture the initial stages of the process and may not show the changes that occur over longer timescales.

- The microstructure imprints were taken with a time gap of 100seconds
- The structure visually appeared same till 1500sec
- For analysis we need longer time durations (24-30hrs) to visualize the change in behaviour
- It requires High computation cost and system requirements
- Also, a video demonstration of real-time model output behaviour has been generated from the simulation frames, which is also time-consuming task for the model
- The simulation model involves performing calculations on a large matrix, which can be computationally expensive.
- The time required to complete the simulation depends on the size of the matrix and the number of iterations performed.
- For a large matrix and a large number of iterations, the simulation can take a significant amount of time to complete.
- Running this model on a normal system is not sufficient for larger simulations or simulations with many iterations.

❖ CONCLUSION

In conclusion, the model is a simple diffusion simulation that can be used to model the oxidation behaviour of metals. The model takes an input image, converts it to grayscale, and simulates the diffusion of oxygen through the metal. The simulation is saved as a video and as individual frames. The parameters of the model can be adjusted to change the behaviour of the

simulation. However, the simulation can be computationally intensive and may require a powerful machine to run efficiently for a large number of time steps. Thus, the model could be further optimized in due course of time and worked on systems with sufficient processing power.

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