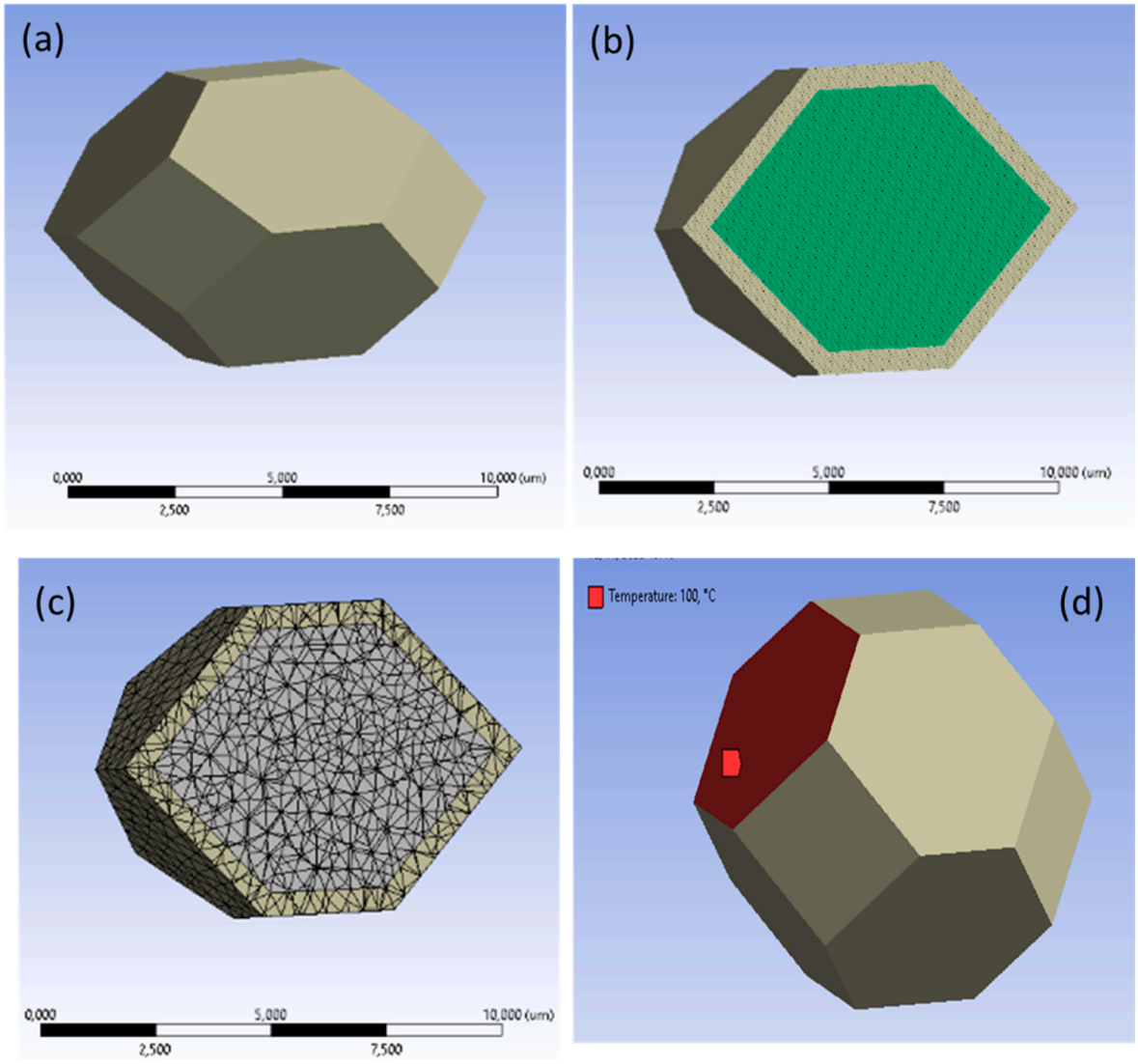

Fig. 8. Geometry of the 3D model (a), mesh of the 3D model (b,c), thermal analysis configuration for the 3D model (d).

Table 5
Mesh statistics for the 3D model.

Meshing parameter	Value
Total number of nodes	29 091
Total number of elements	20 095
Grain number of nodes	15 781
Grain number of element	13 022
Boundary grain number of nodes	13 310
Boundary grain number of element	7073

Table 6
Material properties for the 3D model.

Material Name	Mat ID	Density, ρ [$\frac{kg}{um^3}$]	Specific Heat, cp [$\frac{pj}{kg\,K}$]	Conductibility coefficient, KXX [$\frac{pW}{um^3 K}$]
Lattice	1	1	1	0,00014
Boundary grain	2	1	1	0,14
Dislocation	3	1	1	0,014
Precipitates	4	1	1	0,00014

Table 7
Thermal analysis set-up for the 3D model.

Properties	Step
Step Controls	
Step End Time	2000
Auto Time Stepping	Program Controlled
Time Integration	On
Nonlinear Controls	
Heat Convergence	Program Controlled
Temperature Convergence	Program Controlled
Line Search	Program Controlled
Output Controls	
Contact Data	Yes
Nodal Forces	No
Contact Miscellaneous	No
General Miscellaneous	No
Euler Angles	Yes
Volume and Energy	Yes
Calculate Thermal Flux	Yes
Store Results At	All Time Points
Advanced	
Contact Split (DMP)	Off

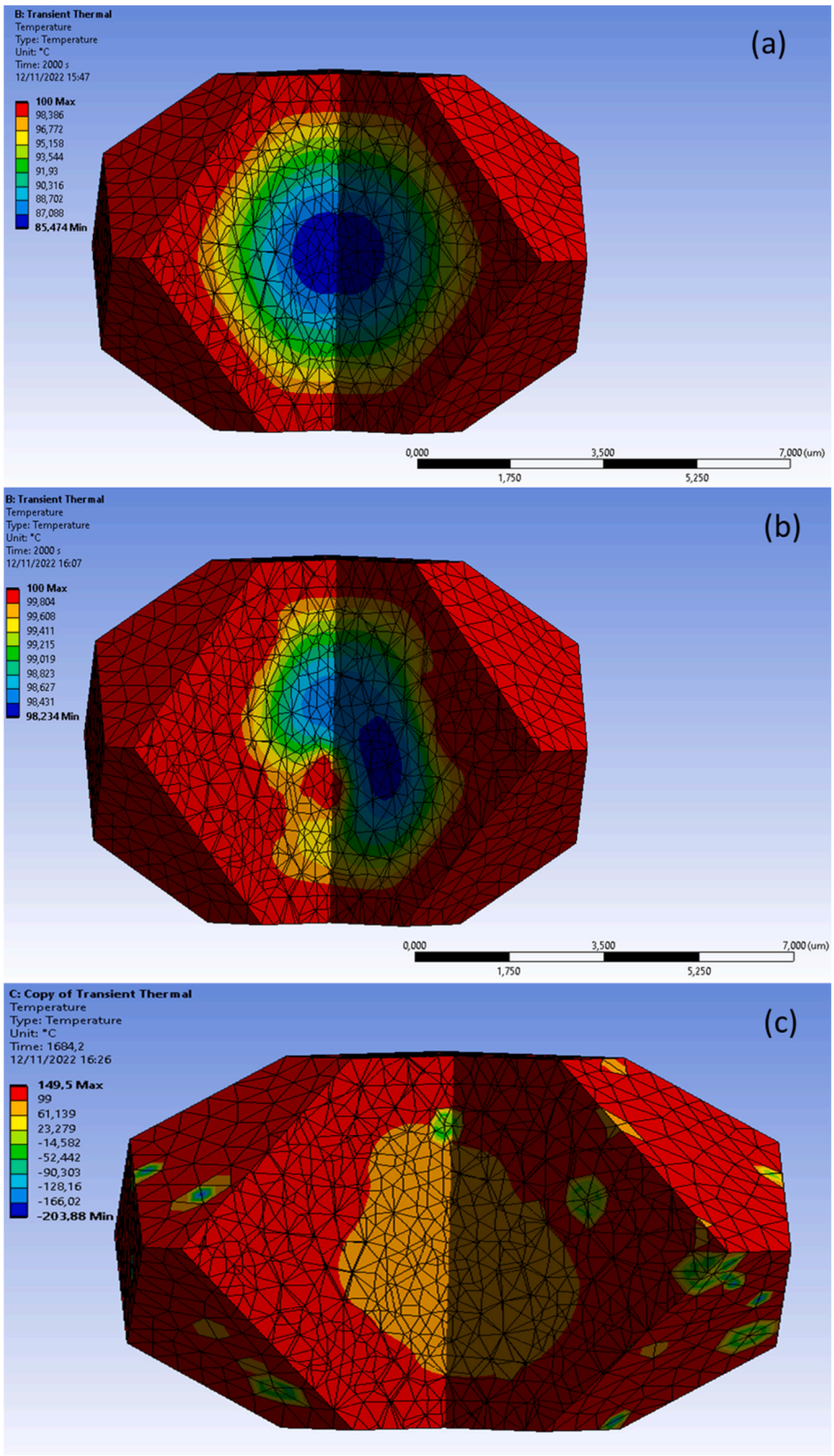

Fig. 9. (a)Thermal analysis nodal results for the 3D model, (b) Thermal analysis nodal results for the 3D model considering the dislocations effect, (c) Thermal analysis nodal results for the 3D model considering the precipitates effect.

the steel and the amount of total area occupied by precipitates by assuming that the precipitates have a spherical shape.

Each type of precipitate is analysed to discover how many atoms of hydrogen can fill it.

In the first type of precipitates there are: Vanadium carbides (*VC*), it's an extremely hard refractory ceramic material. It has a cubic crystal structure whit an Pearson symbol of cF8. The space group is Fm3m. Vanadium nitride (*VN*), it's formed during the nitriding od steel. It has a

Table 8
Dislocation design parameters for the 3D model.

Design parameter	Value
Dislocation density $[\frac{1}{m^2}]$	10^{16}
Dislocation length [pm]	160 000
Number of hydrogen atoms that fill all the dislocations	$5.76 * 10^9$
Dislocation number of elements, N_{disl}	2019

Table 9
Precipitates element calculations for the 2D model.

Type of precipitate	Number of nodes in boundary grain	Number of nodes in grain	Total number of nodes	Total number of elements	Total number of saturated elements
G1	31	14	45	270	270
G2A	80	35	115	690	690
G2B	41	17	58	348	348
G3	10	5	15	90	90

Table 10
3D complex geometry model design parameters.

Design parameter	Value
Total grain volume [um^3]	785.4
Boundary grain thickness [um]	1
Boundary grain volume [um^3]	994.3
Total volume [um^3]	1779.7

cubic crystal structure whit a Pearson symbol of cF8.

These precipitates are formed by Vanadium that is a hard malleable transition metal. Vanadium atoms has an atomic radius of 130 [pm]. Nitrogen has an atomic radius of 65 [pm]. Carbon has an atomic radius of 70 [pm].

The second type of precipitates are formed by Chromium carbides (Cr_3C_2). Cr_3C_2 is a refractory ceramic material. Its crystal structure is orthorhombic.

These precipitates have an average diameter of 100 [nm] The second

Table 11
Geometrical design parameters.

Design parameter	Value
Parallelepiped size [um x um x um]	31 × 31 x 31
Total volume [um^3]	28 668
Average grain volume [um^3]	132,3
Number of grains	164
Total grain volume [um^3]	21 701
Boundary grain thickness [um]	1
Boundary grains volume [um^3]	6967

Table 12
Mesh design parameters.

Mesh parameter	Value
Total number of nodes	1 064 991
Total number of elements	777 753
Grain number of nodes	889 186
Grain number of element	567 995
Boundary grain number of nodes	386 099
Boundary grain number of element	209 758

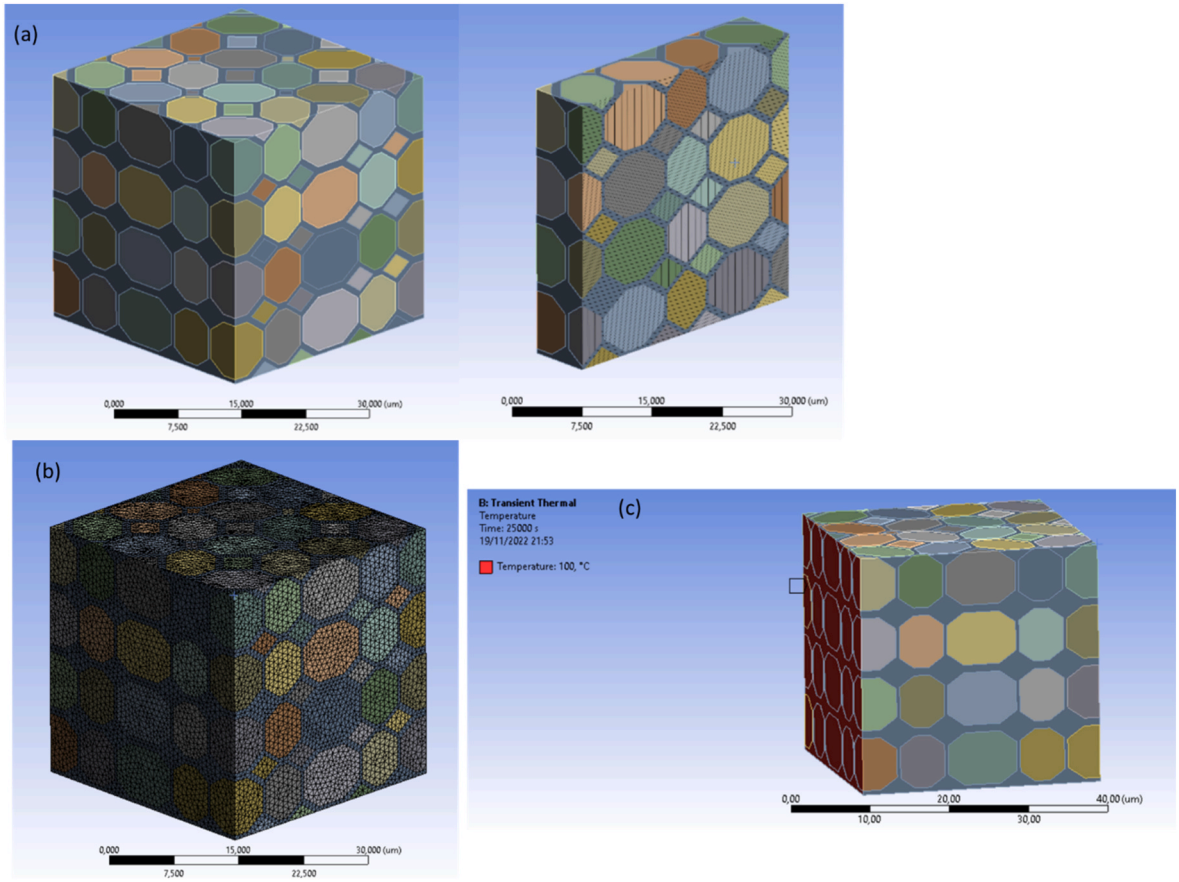

Fig. 10. (a) 3D final geometry, (b) 3D final mesh, (c) Final Model set-up.

Table 13
Materials design parameters.

Material Name	Mat ID	Density, ρ [$\frac{kg}{um^3}$]	Specific Heat, cp [$\frac{pj}{kg\,K}$]	Conductibility coefficient, KXX [$\frac{pW}{um^3K}$]
Lattice	1	1	1	0,00014
Boundary grain	2	1	1	0,14
Dislocation	3	1	1	0,014
Precipitates	4	1	1	0,00014

Table 14
Dislocation Mesh parameters.

Mesh parameter	Value
Dislocation number of nodes	12 956
Dislocation number of element	58 848

Table 15
Final Model simulation settings.

Properties	Step
Step Controls	
Step End Time	25 000
Auto Time Stepping	Program Controlled
Time Integration	On
Nonlinear Controls	
Heat Convergence	Program Controlled
Temperature Convergence	Program Controlled
Line Search	Program Controlled
Output Controls	
Contact Data	Yes
Nodal Forces	No
Contact Miscellaneous	No
General Miscellaneous	No
Euler Angles	Yes
Volume and Energy	Yes
Calculate Thermal Flux	Yes
Store Results At	All Time Points
Advanced	
Contact Split (DMP)	Off

type of precipitates includes Cementite Fe_3C also. Cementite is a metal carbide which has an orthorhombic structure. It is a hard and brittle material.

The last type of precipitates are the smallest precipitates. In this case there are the Chromium nitride whit particle size of 20 [nm], CN has a face-cantered cubic structure.

Precipitates are mostly located around the boundary grans. For this reason, the 70 % of the precipitates will be implemented in the boundary grain geometry. The remaining fraction will be implemented in the lattice.

All the results obtained for the precipitates calculation are reported in Table 3.

2.4. 2D vacancies

Vacancies are characterized by a missing atom in the reticular site. Vacancies can be the result of atomic vibration and its number increase when the temperature increases following the expression (eq. (19)):

$$N_v = N_0 \exp\left(-\frac{Q_v}{RT}\right) \tag{19}$$

Where N_0 is the total reticular site, N_v is the number of vacancies at equilibrium, R is gas constant, Q_v is the activation energy (vibration energy required to from a vacancy) and T is the absolute temperature. In general, for metals, there is a vacancy for 10 000 atoms when the temperature is equal to the fusion temperature.

The number of vacancies in function of the temperature is shown in Fig. 6.

The number of mesh element that have to simulate the vacancies effect is three orders of magnitude lower than that of the other traps, for this reason the implementation of the vacancies is not executed.

After defining the boundary conditions of the problem, the model can be implemented.

2.5. 3D model implementation

The 3D model is implemented following the three steps of the 2D model such as: pure diffusion without traps, dislocation simulation and precipitates simulation.

The second model (3D) is implemented in Ansys Workbench. In the FEM model APDL is used also.

Ansys Workbench is a Finite Element Analysis (FEA) software that is

Table 16
Precipitate calculation results.

Type of precipitate	Number of nodes in boundary grain	Number of nodes in grain	Total number of nodes	Total number of saturated nodes
G1	1210	518	1728	168
G2A	3124	1339	4463	464
G2B	1578	677	2255	334
G3	414	177	591	121

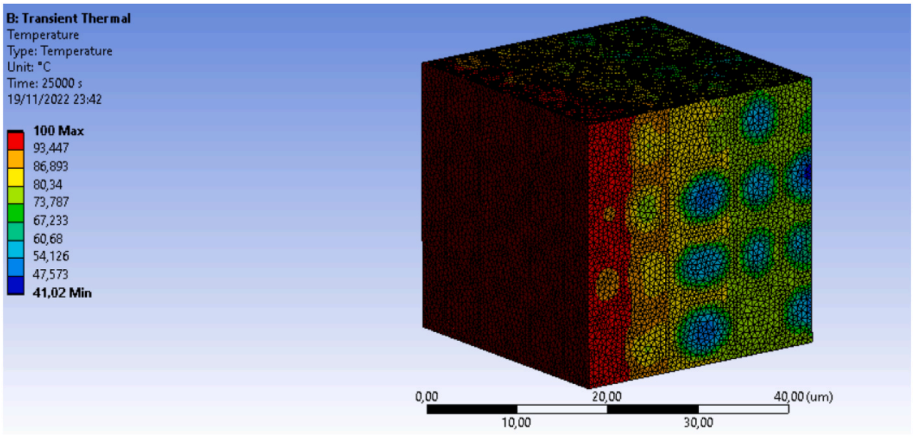

Fig. 11. Element solution result for the Final Model (dislocation implementation).

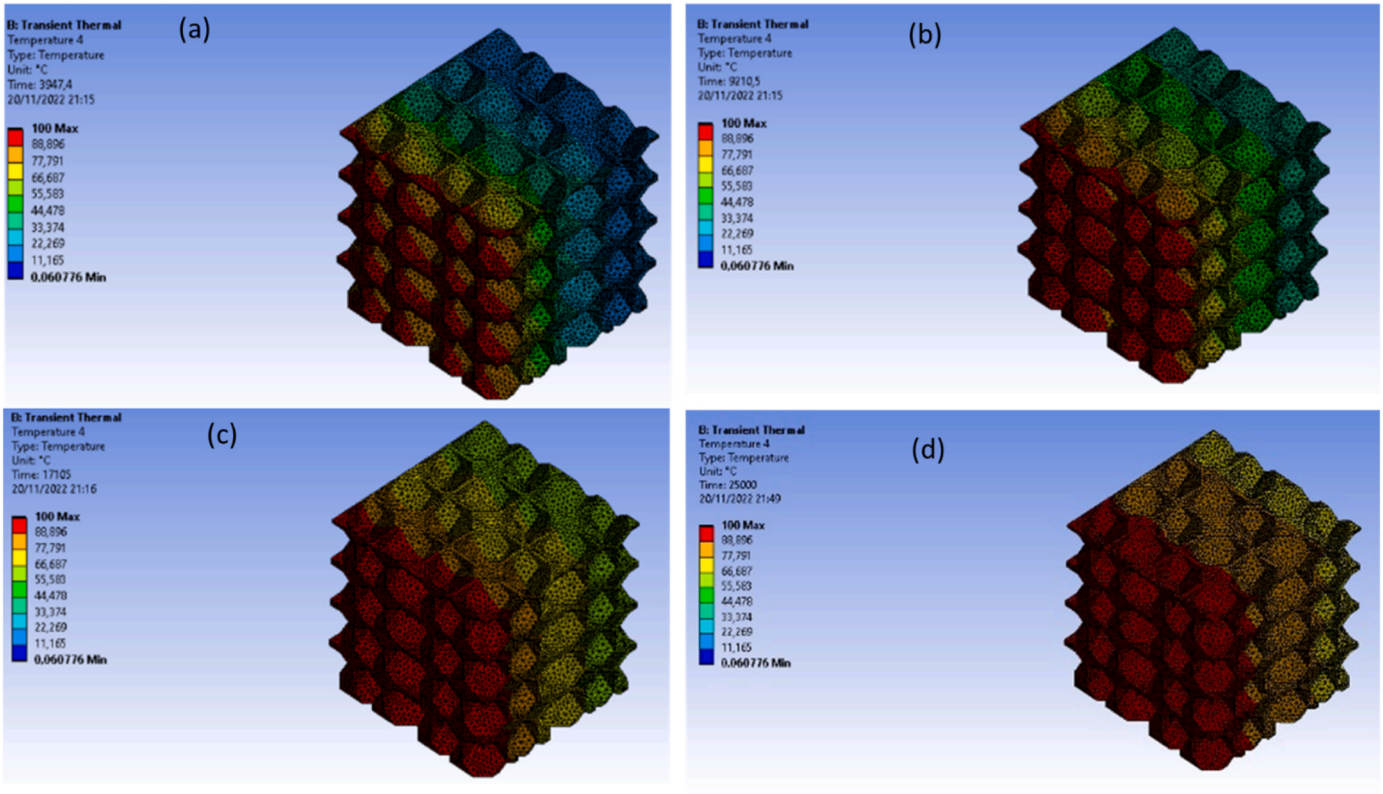

Fig. 12. Grain boundary hydrogen saturation evolution, 4000 s (a), 9000 s (b), 17 000 s (c), 25 000 s (d).

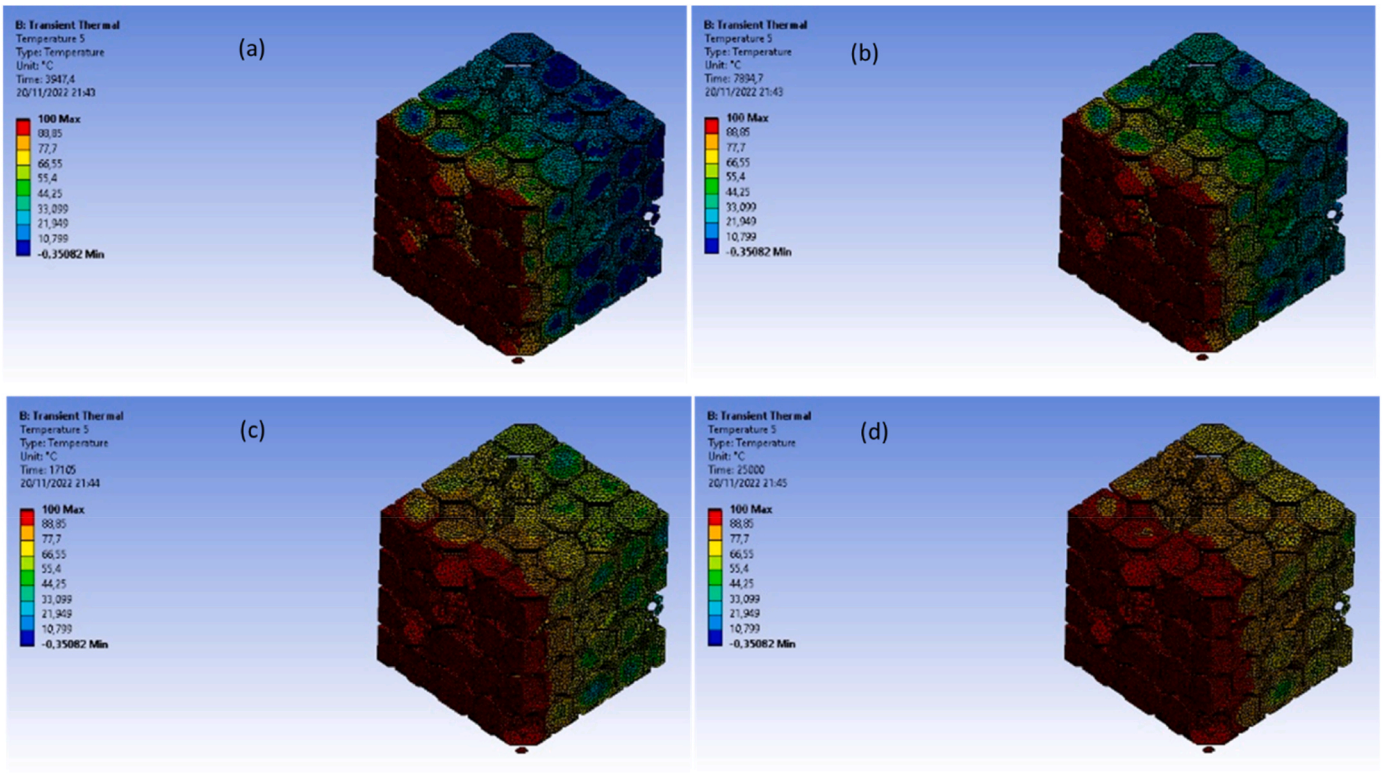

Fig. 13. Grain hydrogen saturation evolution, 4000 s (a), 8000 s (b), 17 000 s (c), 25 000 s (d).

widely used for engineering applications. This tool can simulate problems from different field such as Structural, Vibrations, thermal etc. In this thesis thermal analysis module will be used for the hydrogen diffusion. Ansys Workbench allows to use macros written in APDL to parameterize simulations. Fig. 7 shows the flowchart of the 3D model.

The first model is based on the hydrogen pure diffusion in a

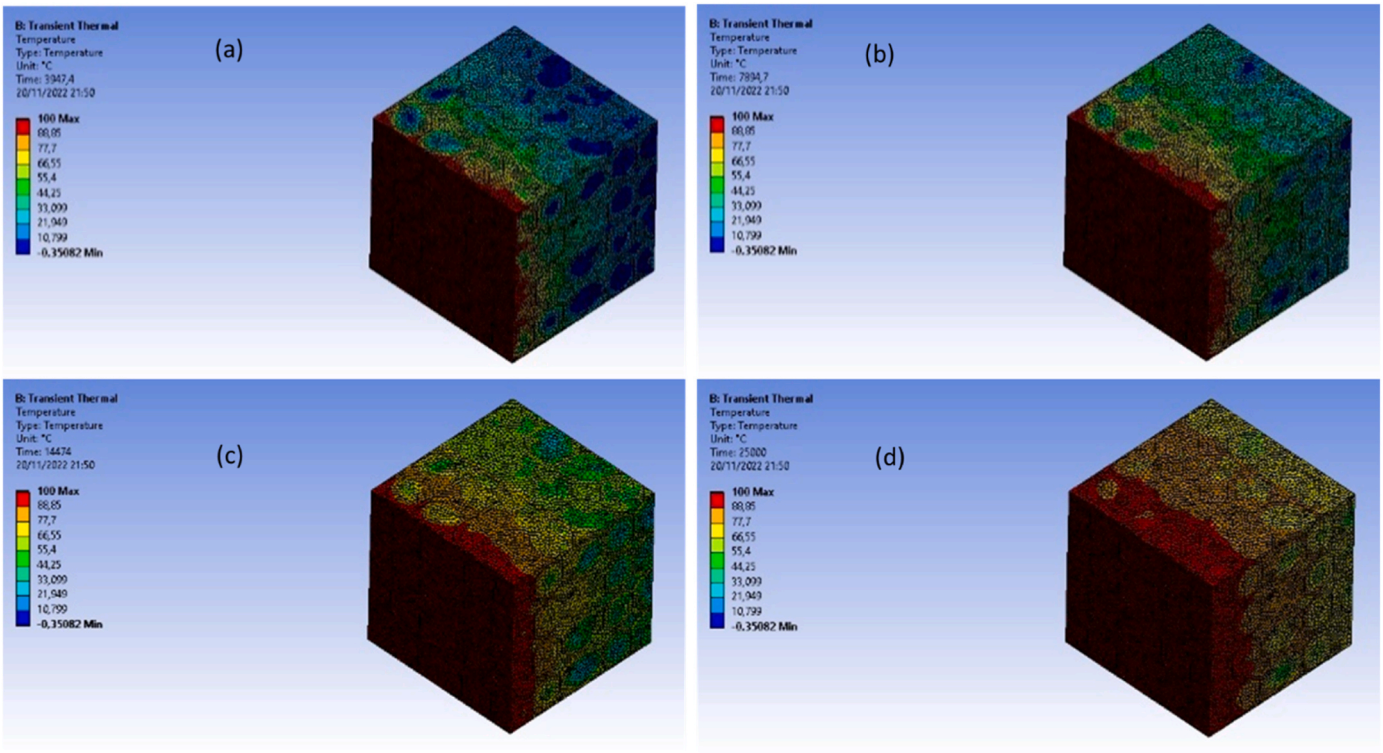

Fig. 14. Hydrogen saturation evolution, 4000 s (a), 8000 s (b), 14 000 s (c), 25 000 s (d).

truncated octagon shape, surrounded by the boundary grain. Boundary grain is the only trap that is implemented in this model.

2.6. 3D geometry and mesh

The microstructure is formed by a truncated octagon grain surrounded by grain boundary phase. The dimension of geometry is reported in Table 4.

Fig. 8(a–c) shows the geometry of the simulated microstructure and the implemented mesh.

It is important that the elements of the mesh have approximately the same size. To obtain a mesh with these properties, the body sizing tool was used. The properties of the mesh are shown in Table 5.

The grain and the grain boundary are characterized by having two different behaviours for the hydrogen diffusion problem, for this reason two different materials are used whose properties are shown in Table 6.

After the meshing process and inserting the properties of the materials, it's possible to proceed with the first 3D simulation.

Also, in this case thermal transient simulation is carried out to simulate the diffusion of the hydrogen. Using the analogy with the thermal problem, it is sufficient to enter a uniform temperature of 100 °C which simulates a saturation of 100 % hydrogen on one face of the truncated octagon. Fig. 8 (d) shows the configuration of the model before the first simulation.

Table 7 shows the setting of the thermal transient simulation.

3. Results and discussion

Fig. 9 (a) shows the nodal solution of the pure diffusion simulation in the first model.

From the nodal solution of the 3D simulation, it's possible to observe that.

1) hydrogen diffuses at different rates depending on the properties of the material used.
2) The maximum concentrations of hydrogen occur in the grain boundary which represents the preferential diffusive path, for this reason grain boundary is completely saturated.
3) In the lattice, the concentration of hydrogen is directly proportional to the distance from the grain boundary, in fact the highest concentrations occur near the edge, while more time of diffusion is required to saturate the lattice core.

The next step concerns the implementation of traps such as dislocations and precipitates.

The first type of trap that will be implemented are dislocations. To calculate the number of elements that will simulate the dislocation, the same approach of the 2D case is used. Table 8 summarized the dislocation calculation for a temperature equals to 300 K.

Knowing the number of elements N_{disl}, it's possible to update the model by adding the material of the dislocation and the dislocation elements.

After the implementation of the new mesh, a new simulation is lunched. The results are shown in Fig. 9(b). From nodal solution of the dislocation simulation, it's possible to observe that.

- Diffusion path in lattice is highly influenced by the dislocation's elements, dislocation accelerate the diffusion in the lattice.
- Boundary grains have still the maximum hydrogen concentration.
- Hydrogen concentration in lattice is still dependent on the distance from the boundary grain, but the dependence from dislocation effect is greater. This consideration is due to the fact that the saturation of the grain is strongly asymmetry.

The last type of traps that is analysed are the precipitates. To calculate the number of elements that will simulate the precipitates, the same approach of the 2D case is used.

Since precipitates are irreversible traps, it is necessary to know how many of these traps are saturated. To solve this problem, macros have been implemented that analyze the concentration of hydrogen before the generation of precipitates. If the hydrogen concentration is higher