ORIGNAL PAPER

X-RAY DIFFRACTION STUDY OF THE CRYSTAL STRUCTURE OF HASTELLOY C2000 BETWEEN 700°C AND 1000°C

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Abstract. *Hastelloy C2000 is a superalloy used in the chemical processing, pollution control and waste treatment industries. This alloy contains a nominal amount of 52-60% of Ni, 15-31% of Cr, 9-16% of Mo, and small additions of other elements such as iron, copper, tungsten, etc. Its matrix is austenitic and its structure is face-centered cubic.*

The objective of our work is to study the structure of the Hastelloy C2000 and this by a heat treatment at four temperatures: 700 °C, 800 °C, 900 °C and 1000 °C with a prolonged maintenance at each temperature during three hours. The monitoring of the structure is performed by using the X-ray diffraction (XRD).

The X-ray diffraction spectra obtained after the heat treatments, show the presence of peaks of the precipitates and the peaks of the austenite phase. For the crystallographic parameters of the mesh before and after the four heats treatments, we remark an increase of the parameter a and the volume of the mesh as a function of treatment temperature.

Keywords: *Hastelloy C2000, Structure, X-Ray Diffraction, heat treatment, crystallographic parameters.*

1. INTRODUCTION

In many fields of industrial activity (chemical reactors, thermal power plants, aeronautics, automotive, coal gasification, heat treatments, etc.), the choice of materials used must take into account their mechanical, structural properties and their corrosion resistance and this is more interesting when they are subjected to the increase of the temperatures and to the complexity of the working environments.

Since the discovery of X-rays in 1895 by WKRotgen [1], and because of the inventions relating to experimental techniques, methods of analysis and theoretical developments, the X-ray diffraction (XRD) technique is widely used to characterize and understand the crystallographic structure of the crystalline materials, their texture and associated microstructure [2-3].

The application of X-rays to the case of nickel-based austenitic stainless steels, specifically to Hastelloy C2000 steel, is the objective of our structural investigation carried out during our study and this for four temperatures: 700°C, 800°C, 900°C and 1000°C.

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2. MATERIALS AND METHODS

2.1. X-RAY DIFFRACTION

The X-ray diffraction spectra of the four samples treated are obtained at ambient temperature using a D2 PHASER diffractometer of Bragg-Brentano focusing geometry with a Cu Ka radiation type = 1.5406 Å. The data are recorded over a range of 2θ between 10 and 100 ° with a pitch of 0.01 (2θ).

The determination of the positions of the diffraction lines and the relative intensity of the peaks, which was determined from the height of the peaks above the continuous bottom, was realized by using the WINPLOTR software.

3. X-RAY DIFFRACTION ANALYSIS OF HASTELLOY C2000 ALLOY BEFORE TREATMENT

In X-ray diffraction, the basic information which is essentially processed is the diffraction lines. The fine line analysis allows us to access to two categories of information: position and intensity (area of the diffraction line) [4].

The Fig. 1 represents the diffractogram obtained before treatment of the alloy Hastelloy C2000. According to the diffractogram, the structure of the alloy is monophasic, characterized by the (111), (200), (220), (311) and (222) planes determined from the ASTM plugs. We also note that the peaks at positions (a), (b), (c), (d) and (e) are singlets before treatment.

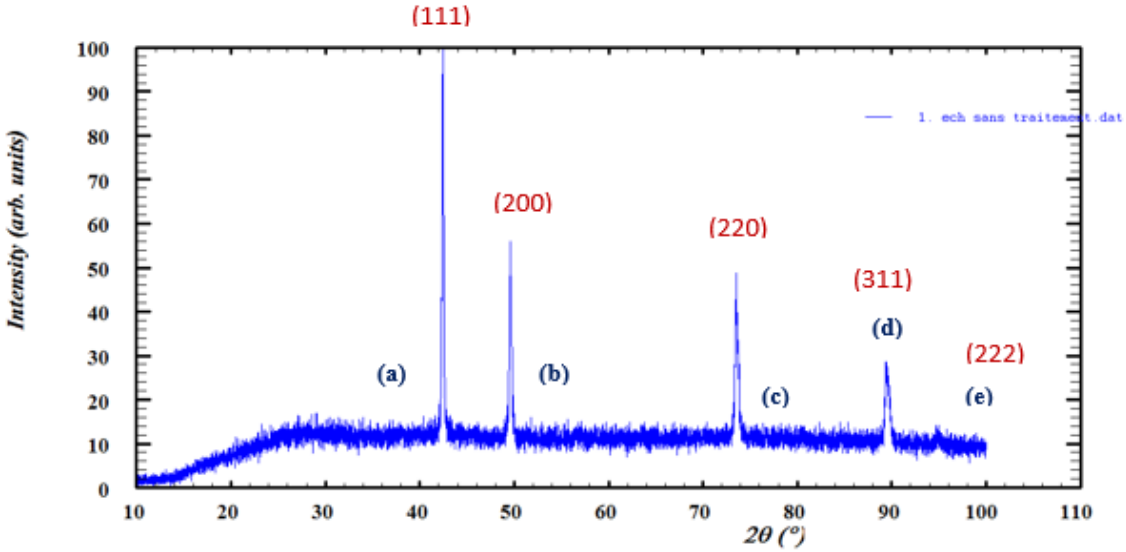

Figure 1. X-ray diffraction spectrum of the C2000 alloy before heat treatment.

The Table 1 summarizes the results obtained using the WINPLOTR software for the Hastelloy C2000 alloy before treatment. As shown in the table, for the structure, it is orthorhombic with a ≠ b ≠ c with a volume of 24.25 $Å^3$.

Table 1. Parameters of the mesh of the alloy Hastelloy C2000 before treatment.

a (Å)	b (Å)	c (Å)	V (Å^3)	α	β	γ	parameters	structure
3.5727	2.6633	2.5531	24.25	90	90	90	$a \neq b \neq c$ $\alpha = \beta = \gamma$	Orthorhombic

4. INFLUENCE OF THE HEAT TREATMENT ON THE STRUCTURE OF THE HASTELLOY C2000

The Fig. 2 shows that the X-ray diffraction spectra of the four pieces treated at 700 °C, 800 °C, 900 °C and 1000 °C are similar. Consequently, the structure of this alloy treated at these four temperatures remains monophasic.

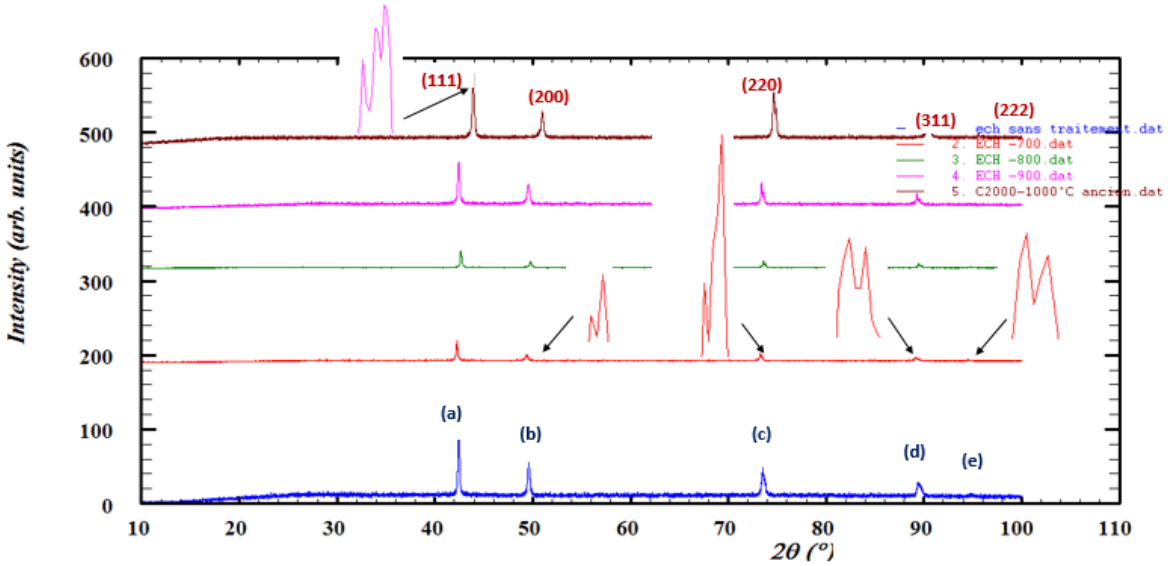

Figure 2. X-ray diffraction of the C2000 alloy of the pieces treated at 700 °C, 800 °C, 900 °C and 1000 °C, after 11 days of quenching.

According to the ASTM sheets, it can be deduced that this structure is characterized by the (111), (200), (220), (311) and (222) planes also found for the same type of alloy studied by Huang [5]. The positions (a), (b), (c), (d) and (e) became, after treatment, a doublets for the piece treated at 700 °C and triplets for the other pieces treated at 800 °C, 900 °C and 1000 °C which correspond to the austenite phase and precipitates.

We also notice that when we increase the temperature of the treatment, the intensity of peaks increases and this is due to rearrangements of the positions of atoms. However, the intensity of the Bragg peaks is directly proportional to the increase in the volume fraction of the growing phase [6] and this agrees with the results found for the parameters of the mesh as a function of the temperature of the heat treatment.

For the diffraction spectrum, which corresponds to the piece treated at 1000 °C, we notice that it has a movement of peak in the position (a) compared with the peak of the untreated piece. This displacement can be attributed to elastic deformation of the crystal lattice. Indeed, the deformations of the crystal lattice are related to the diffractive nails by the Bragg relation [7].

The Fig. 3 corresponds to the X-ray diffraction spectra of the four pieces treated at 700 °C, 800 °C, 900 °C and 1000 °C obtained two months after quenching. We note that the peaks are similar to those obtained 11 days after the quenching just for the piece treated at 1000 °C, there is an increase in the intensities of the peaks. This elevation may be due to the grain morphology, which changes significantly as a function of time. This phenomenon was also encountered for another type of stainless steel [8].

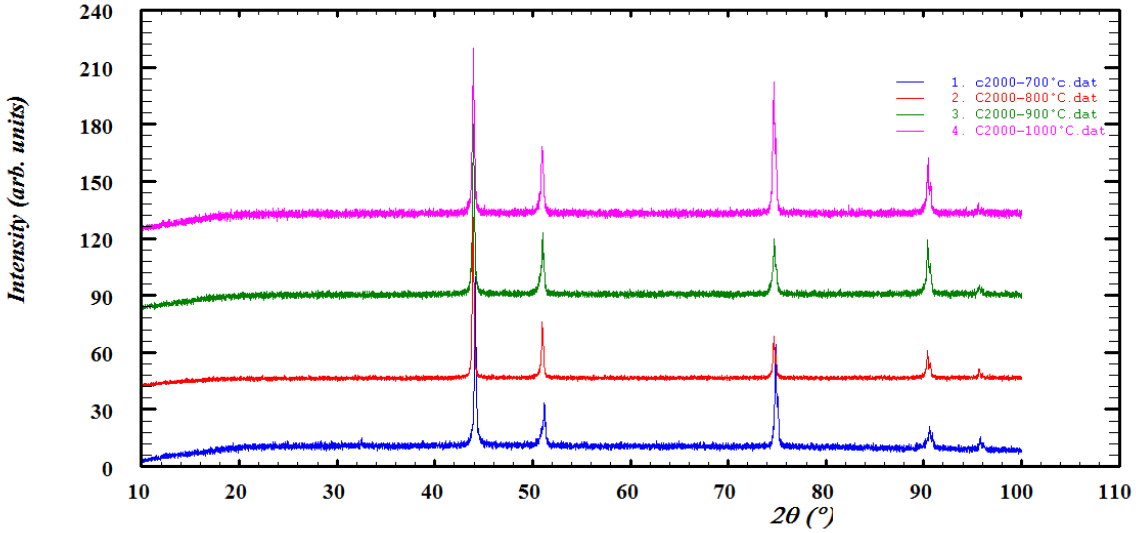

Figure 3. X-ray diffraction of the C2000 alloy of the pieces treated at 700 °C, 800 °C, 900 °C and 1000 °C, after 2 months of quenching.

5. CALCULATION OF THE MESH PARAMETERS

To calculate the parameters of the mesh, for each treatment temperature and based on the given inter-particle distance from the difractogram, we used the following relation in the case of a cubic crystal system:

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \qquad (1)$$

with : d_{hkl} : interreticular distance (Å) ;
a : parameter of the mesh (Å) ;
h,k,l : reticular planes.

The Table 2 lists the crystallographic parameters of the Hastelloy C2000 for the treatment temperatures 700 °C, 800 °C, 900 °C and 1000 °C. According to the table 2, we notice that the average values found of the parameter (a) are close for the various temperatures of the treatment. The average value of the results found of the parameter (a) is 3.5835 Å.

Table. 2. Crystallographic parameters of the HASTELLOY C2000 treated at 700 °C, 800 °C, 900 °C and 1000 °C.

T=700 °C			**T=800 °C**		
d(hkl) en (Å)	hkl	a (Å)	d (hkl) en (Å)	hkl	a (Å)
2.0506	111	3.5517	2.065	111	3.5767
1.7827	200	3.5654	1.7897	200	3.5794
1.2670	220	3.5836	1.2697	220	3.5913
1.0928	311	3.6244	1.0853	311	3.5995
1.0343	222	3.5829	1.0259	222	3.5538
Moyenne de a (Å)		3,5816	Moyenne de a (Å)		3.5801
T=900 °C			**T=1000 °C**		
d(hkl) en (Å)	hkl	a (Å)	d(hkl) en (Å)	hkl	a (Å)
2.0589	111	3.5661	2.0583	111	3.5651
1.7881	200	3.5762	1.7900	200	3.5800
1.2691	220	3.5896	1.2698	220	3.5915
1.0851	311	3.5989	1.0850	311	3.5985
1.0426	222	3.6117	1.0343	222	3.5829
Moyenne de a (Å)		3.5885	Moyenne de a (Å)		3.5836

The Table 3 groups the crystallographic parameters of the mesh obtained, by the software WINPLOTR, for each temperature of treatment.

Table. 3. Parameters of the mesh of the HASTELLOY C2000 treated at 700 °C, 800 °C, 900 °C and 1000 °C.

T (°C)	**a (Å)**	**b (Å)**	**c (Å)**	**V (Å^3)**	**α**	**β**	**γ**	**parameters**	**structure**
700	3.5926	3.1208	2.7195	30.49	90	90	90	$a \neq b \neq c$ $\alpha = \beta = \gamma$	Orthorhombic
800	3.6033	3.5423	2.5414	32.44	90	90	90	$a \neq b \neq c$ $\alpha = \beta = \gamma$	Orthorhombic
900	3.6107	3.5800	2.5031	32.62	90	90	90	$a \neq b \neq c$ $\alpha = \beta = \gamma$	Orthorhombic
1000	3.6212	3.1242	2.7631	33.07	90	90	90	$a \neq b \neq c$ $\alpha = \beta = \gamma$	Orthorhombic

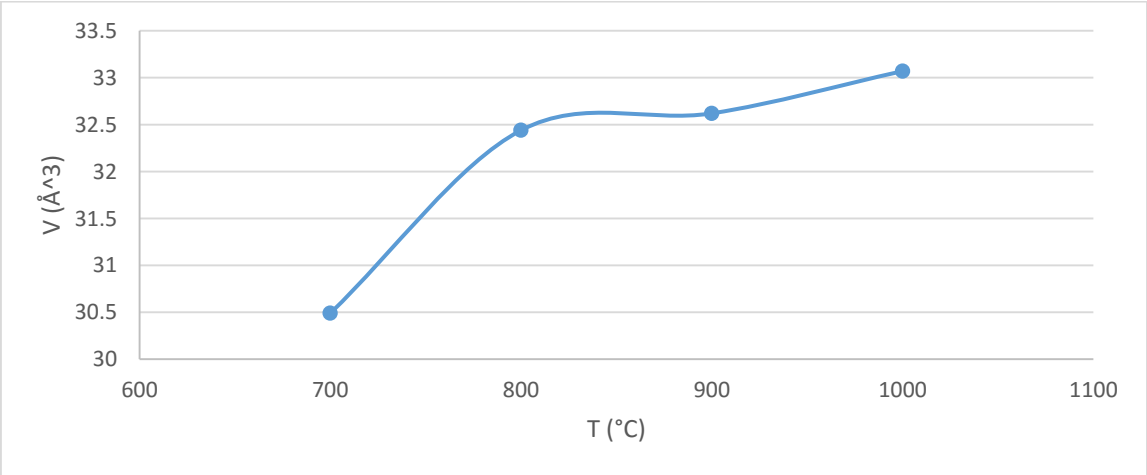

Figure 4. Variation of the volume of the mesh of the Hastelloy C2000 as a function of temperature.

The structural study (Table 3) as a function of the heat treatment temperatures reveals an increase of the parameter (a) and the volume of the mesh (Figs 4 and 5). Therefore, the size effect already observed in previous studies [9-11] is strongly correlated with a modification of the crystalline parameters. For the structure, it remains orthorhombic for the different temperatures of the treatment.

Indeed, for the temperature of the treatment 1000°C, the rate of increase of the volume of the mesh is 36.37%.

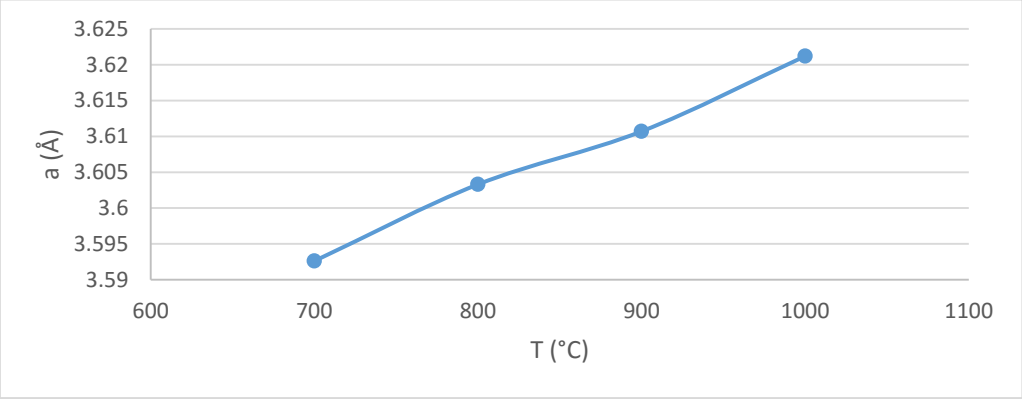

Figure 5. Variation of the mesh parameter a of the Hastelloy C2000 as a function of temperature.

6. CONCLUSION

In this work, the Hastelloy C2000 was treated for 3 hours at four different temperatures: 700 °C, 800 °C, 900 °C and 1000 °C. We deduce that an increase in temperature makes possible to improve the intensity of the peaks; this is due to rearrangements of the positions of the atoms. For High temperatures (1000°C), we notice also a displacement of peak; this is due to an elastic deformation of the crystal lattice. We remark also an increase in the intensities of the peaks, for the same piece treated at 1000°C, 2 months after quenching. This elevation may be due to the grain morphology, which changes significantly as a function of time. The structural study of the Hastelloy C2000 as a function of the different treatment temperatures shows that the mesh parameter increases from 3.5727 Å (before treatment) to 3.6312 Å after treatment (at 1000 °C). The crystal structure remains orthorhombic; it does not depend on the temperature of the treatment.

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