Towards a smart simulation of surface modification by thermochemical treatments for stainless steel in the industrial revolution 4.0

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Abstract. This paper provides a conceptual basis of the development of a virtual process control design using smart simulation in the thermochemical surface engineering design for stainless steel. A historical review as a foundation of further development in attaining a smart simulation on low temperature thermochemical treatments is highlighted. Both scientific platforms and commercial explorations are suggested to thoroughly study the possibility of attaining a smart simulation on this material manufacturing related field. It is concluded that three essential stages of future works need to be performed: the construction of base points, model and simulation development, and advancement of simulation related to additive manufacturing to create a smart simulation in the industry 4.0 era.

1. Historical perspective
Stainless steel is a group of metallic materials used in various kinds of industrial need. It was firstly invented by Harry Brearley, a metallurgist from Sheffield, UK, in 1913 [1]. A wide range of application of this material can be found everywhere, from domestic appliances, chemical industries, building structures, transport equipment, jewelries, medical equipment, and nowadays for surgical implanted parts. Stainless steel is one of the most commonly used biomaterials as internal fixation due to a great combination of its mechanical properties, biocompatibility, corrosion resistance and cost effectiveness [2].

The world’s annual production of stainless steel has consistently increased over the last 50 years’ period [Figure 1], thus demand for this material has continuously increased in various sectors of applications. The austenitic type of stainless steel constitutes around 70% of total stainless steel demand, with China being the highest producing country [Figure 2]. Regardless of its advantages pertaining to good manufacturability and a lower price, the austenitic type of stainless steel has the lowest values in hardness and wear resistance in comparison to other types of stainless steel.
Efforts were made to improve the surface mechanical properties of the austenitic stainless steel in the early 1980’s. The earliest publication on the surface modification of austenitic stainless steel was made by previous works [4-6]. The technique involved nitriding in a glow discharge assisted atmosphere or namely plasma nitriding to improve the surface hardness of the material. Improvement in the surface hardness was found to be five times significantly above the hardness of the untreated austenitic stainless steels substrate. Scientific evidence showed that surface hardness improvement was caused by the formation of expanded austenite, or identified as S-phase, formed in the nitrogen diffusion zone with thickness that depends on the treatment time [8-10].

Despite the marked improvement on the surface hardness of austenitic stainless steel AISI 316L, such investigations showed that the treatment causes a deterioration effect to the corrosion resistance of this material due to chromium depletion in the solid solution by forming CrN precipitates and consequently leading to a sensitivity to intergranular corrosion attacks [11]. Only after the nitriding treatment was performed below 500 °C the resultant nitride layer was free from nitrogen precipitation. These thermochemical treatments applied for stainless steel is technically termed as low temperature thermochemical treatment [12].

The development in low temperature thermochemical treatment in the early stages [1985-2000] was marked by various publications in exploring the characteristics of expanded austenite layers mostly produced by plasma nitriding and carburizing techniques [13]. The understanding of the physical
metallurgy of S-phase or expanded austenite involving both nitrogen and carbon in low metastable solid solution was the main focus of research interests during that period.

In that period of time, various glow discharge techniques such as RF discharge, DC diode, plasma immersion ion implantation, low pressure plasma, and ion beam processing were the main attractions of investigations. Other surface modification techniques by solution nitriding [14], salt bath nitriding [15] and gaseous carburizing [16] were also studied with regard to their feasibilities and in agreement with precise control techniques using glow discharge assisted atmosphere.

A number of research works from various parts of the world, shown in Table 1, were conducted to investigate the development of the thermochemical treatments. But only after the year 2005, low temperature nitriding became available for commercial applications. This excellent contribution by the international research communities in this specific area of surface heat treatments provided a sound scientific basis and technological solution to a required industrial need in the current progressive decade.

Table 1. World’s research works

| Year | Country          |
|------|------------------|
| 1985 | United Kingdom   |
|      | Germany          |
|      | Denmark          |
| 1990 | Denmark          |
|      | Korea            |
|      | Japan            |
|      | Australia        |
| 2005 | Malaysia         |
|      | Singapore        |
| 2010 | Brazil           |
| 2012 | Iran             |
| 2014 | Mexico           |
| 2018 | Indonesia        |

Following the early years of research work, an introduction of hybrid thermochemical treatment was published [17] in which nitrogen and carbon are simultaneously diffused into the surface of stainless steel at temperatures below 500°C. As a result of this combined diffusion, a thick hard layer with smooth hardness gradient in the region adjacent to the layer-substrate interface were produced [Figure 3] thus providing a superior load bearing capacity than that resulted from individual nitriding and carburizing [18].
In the most recent years, thermochemical treatments to improve surface properties of stainless steel were also studied and was implemented to the duplex type of stainless steel [19]. The works using laboratory gaseous furnace showed that although the hardness of duplex stainless steels improved, difficulties were found in obtaining a thick layer of expanded austenite phase owing to the presence of ferrite phase in the structure. In the case of a hybrid process, the treatment did not produce a dual separate layer consisting of nitrogen expanded austenite (S_N-phase) on top and followed by carbon expanded austenite (S_C-phase) below it, as it was compared to layer formation on austenitic stainless steel surfaces. Figure 4 shows a comparison of resultant layers produced by thermochemical treatments for austenitic stainless steel and for duplex stainless steel.

The surface modification technologies of stainless steels in the explanation above are still the main attraction in the laboratory investigations done for further improvement associated with their commercial availability in industries. These technologies are finding a rapidly expanding niche market covering applications of human needs.

Today in the period of Industry 4.0, after three decades of research development in surface modification of stainless steel, the thermochemical treatments are feasible to be advanced by the usage of mathematical models, simulation, and optimization using computer assisted programming. This virtual technological approach may become a novelty for not only metallurgical related sciences but also for the innovation of additive manufacturing technologies to promote cost effectiveness particularly in manufacturing process design.

Figure 3. Typical hardness profiles resultant from various low temperature plasma surface alloying processes [17].
Figure 4. Comparison of the resultant layers produced by thermochemical treatments for (a) austenitic stainless steels [17] and (b) duplex stainless steels [19].

2. Mathematical model and simulation
A mathematical model of thermochemical treatment was initially carried out for nitriding of low alloy steel by glow discharge technique [20]. The model performed mathematical formulations for various diffusional reactions to represent a complete model of nitriding and used a numerical solution to solve the model. The developed model was used to predict the distribution of nitrogen in solution and in the form of alloy nitride precipitates, the iron nitride layer thickness developed during plasma nitriding, the incubation time for the formation of iron nitride layer, and the nitride precipitation behavior of various alloying elements in the steel. It was concluded that the precision of the calculation results was strongly influenced by the accuracy of diffusion coefficient in various phases and the sputtering rate. The model however had a limitation that it only considered iron-alloy elements systems, whilst the influence of carbon in the substrate and reaction of excess nitrogen, as well as redistribution of carbon and carbides, were not included, hence the accuracy of the model was rather ambiguous.

Modifications of the above model were further proposed by other works [21,22]. In these two modified models, the diffusional coefficient of nitrogen across the diffusion layer was considered independent of the nitrogen content and can be applied to two-phase systems or more. But the models did not consider the impeding effect of dispersed nitrides on the overall diffusive flux of nitrogen. Corrections to the above models were then made by another work [23]. This adapted version of the nitriding model considered system was a continuous and single-phase system because the transition from the expanded austenite to the expanded austenite bulk was caused by the dissolution of nitrogen into the austenite lattice. The work also demonstrated that a strong concentration dependency exists for nitrogen diffusion with a case of expanded austenite stainless steel. The model therefore incorporates a compositional dependent diffusion in the austenitic phased stainless steels. This work however did not include the lattice distortion effect created by interstitial diffusion of nitrogen in the austenite phase during a diffusional process. Thus, the accuracy of the model was not considerable, and a more descriptive model needs to be developed. In the most recent work, the influence of lattice distortion was already considered by which the interaction between the composition-induced stresses and the diffusion was examined for both purely elastic and elastic–plastic stresses [24]. By taking the above considerations in nitriding [19-23], a hypothetical illustration of the mathematical model that can be utilized as a basal platform of further development in obtaining precise calculations for a simulation design on thermochemical treatments of stainless steels is given in Fig. 5. A more delicate mathematical computation might be expected to obtain a precise model for thermochemical treatments of stainless steels due to various parameter effects involved in the process.

Numerous computer software to simulate the manufacturing processes have been established [25, 26]. Simufact and Sorpas are two examples of commercial software that provide process design and simulation on forging and welding in manufacturing operations. In the view of thermochemical
treatments for stainless steels the work on a computer simulation for this manufacturing related field has not been initiated elsewhere. The technological innovations driven by the advancement in artificial intelligence and cloud computing extends the opportunities to implement this information technology basis to the intelligent manufacturing. This will include surface properties enhancement and, in this particular interest, is the simulation of surface modification of stainless steels by thermochemical treatment methods. Such capabilities on applying the conceptual design into a valid simulation, for example the components with a choice of applications, and complementing the experimental research works with the virtual works of simulation, are the challenges to be resolved in order to attain a smart simulation.

![Mathematical Model Process](figure5.png)

**Figure 5. Mathematical Model Process.**

3. **Future works**

Modeling and simulation of the process control in manufacturing operations have long been performed by use of numerical method analysis using computer assisted programming tools. Multi-disciplinary knowledge is needed to resolve complexities that arise in transformation of the physical and metallurgical phenomena to mathematical solutions and to process design simulations. This is the mutual practice that embraces the involvement of materials scientists, manufacturing engineers, as well as mathematicians. In developing the technological establishment of industry 4.0, the contribution of informatics engineers to translate mathematical domains into a virtual simulation becomes a key factor that results in a smart simulation with several user-friendly features. In view of present surface engineering for enhanced wear properties of stainless steels materials, such features like designing the process controls by a combination of working temperatures and treatment durations in a given treatment atmosphere to achieve a superior surface hardness with precision case depth are the main focus of simulation software development. Fig. 6 is a diagram that proposes the future works to be performed in connection to surface modifications of stainless steels by thermochemical treatments.

There are three essential stages that should be considered for the development of a smart simulation. These include construction of the base points, model and simulation development, and advancement of simulation. The four activities contained in the base points represent the need of balanced studies on both technological push factors and business pull factors. In the stage of model and simulation development, the controlling factors in achieving a smart simulation are the complete data of the base point activities. The third stage suggests the possibility of the simulation to be integrated with the
additive manufacturing operations as a finishing step for the enhancement of surface integrity for the stainless steels’ components. In the period of Industry 4.0 applying cloud computing to enable space less and flexible process controls will be the next stage in the development of smart simulation for additive manufacturing operations.

**Figure 6.** Future Works Diagram.

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