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# Hydrogen embrittlement of a Fe–Cr–Ni alloy: Analysis of the physical and chemical processes in the early stage of stress corrosion cracking initiation

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#### ABSTRACT

The interaction of two-hydrogen atoms in a zone of  $\gamma$ -Fe<sub>55</sub>Cr<sub>25</sub>Ni<sub>20</sub> alloy having a vacancy (V) was studied by the atom superposition and electron delocalization molecular orbital (ASED-MO) method. The impurities are located aligned both along [1–10] direction and with the vacancy, in the (111) plane. This behavior can be related with a lineal hydrogen–vacancy clusterization, as a precursor to crack initiation. The electronic structure of the Fe, Cr and Ni atoms near the vacancy, changes after hydrogen's location. The interactions mainly involve Fe 4p<sub>x</sub> and Cr 4p<sub>y</sub> atomic orbitals. The  $3d_{x^2-y^2}$ ,  $3d_{z^2}$  and  $3d_{xz}$  metallic orbitals also have participation in the hydrogen–alloy interactions. An electron transfer to the H atoms from the Fe, Cr and Ni nearest neighbor atoms contributes to form the new H–metal bonds. The metal–metal bonds weakened as the new H–Fe, H–Cr, and H–Ni pairs were formed. The Cr atoms have an important role in the embrittlent process; the strengths of the Cr–Fe, Cr–Cr and Cr–Ni bonds are the most affected while the H–Cr interaction has the highest overlap population. Same H–H interaction is observed and could be associated with the precursor of hydrogen bubble but it is far away to a typical H<sub>2</sub> chemical bond. All the cited physical and chemical processes play a key role in subsequent localized corrosion nucleation such as the initiation of stress corrosion cracking.

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## 1. Introduction

It has long been recognized that the introduction of atomic hydrogen into metallic alloys causes the metal to become embrittled. The embrittlement is often manifested by a significant increase in the ultimate tensile strength and work-hardening rate and a reduction in the strain to fracture [1]. Due to the engineering importance of this problem, a great deal of research has been directed at determining the conditions under which embrittlement occurs and in quantifying the effects.

Molecular dynamics and the embedded-atom method (EAM) have been applied to the study of intergranular hydrogen embrittlement in Ni–Cr–Fe alloys. The simulations suggest that hydrogenembrittlement susceptibility is strongly linked to grain-boundary structure. Boundaries possessing large gaps and structural irregu larities affected adversely, while boundaries lacking these defects are resistant to embrittlement [2].

The initiation of stress corrosion cracking (SCC) in FCC Fe–Cr–Ni ternary alloys was studied by means of quantum chemical molecular dynamics at 288 °C. This study showed that the iron and chromium atoms segregate faster than nickel atoms at the surfaces. The deeply diffused hydrogen becomes negatively charged by taking electron from metal atoms. Consequently, the process weakens the metallic bonds. This kind of reaction process can take place in the molecular domain of a crack tip and thus play a vital role in initiating the SCC process [3].

An internal friction peak due to hydrogen in  $Fe_{55}Cr_{45-x}Ni_x$ (x = 20-45) and  $Fe_{100-x}Ni_x$  (x = 35-100) alloys was observed. A gas-equilibration method was employed in order to charge specimens homogeneously with hydrogen. In  $Fe_{55}Cr_{45-x}Ni_x$  alloys, the peak height significantly increased as the nickel content increased, whereas in  $Fe_{100-x}Ni_x$  alloys the peak height did not show a monotonic change versus the increasing nickel content. In both alloys the peak height depended strongly on the alloy composition [4].

Using the isotope tracer technique, it was observed that microscopic voids artificially induced in Fe–Cr–Ni alloys captured



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tritium. The pressure theory, which is one of the theories concerning failure of iron chromium–nickel alloys, was confirmed [5].

The petrochemical industry has been using cast steel of the 25% Cr-20% Ni type (HK type steel) since the early 1960s in reformer and pyrolysis furnaces. This class of steel had replaced the traditional superallovs with a reduction in costs and has similar properties under conditions of creep, which is one of the principal degradation mechanisms leading to failure in service at elevated temperature. A number of studies were conducted subsequently to evaluate of phase changes during service and the influence of these changes on the mechanisms of failure by creep [6,7]. In the 80s, HP (25Cr/35Ni) modified alloys were developed by using certain metals such as molybdenum, niobium, tungsten, titanium. The problem that was encountered with these materials is severe inservice embrittlement. One factor which can influence the serviceability of reformer tubes is the deficiency in the reformer tube material in terms of mechanical properties, inherent defects [8]. It is well known that defects such as vacancies, act as traps for the hydrogen [9], however, very little is known about the mechanisms by which embrittlement occurs.

In order to study the problem in detail, it is necessary to use computer-simulation techniques which can investigate events on a much finer space and time scale than can be reached with presently available experimental techniques. Analysis of the Fe–Cr–Ni ternary cluster by computational study can provide a fundamental level of understanding for SCC initiation. The purpose of this work is to computationally investigate the physical and chemical processes in the early stage stress corrosion cracking initiation and thus develop a better understanding of the hydrogen embrittlement phenomenon of  $Fe_{55}Cr_{25}Ni_{20}$  industrial alloys.

# 2. Computational method and model

Approximate solutions to Schrodinger's equation are applied to determine the distribution of electron density throughout the model and the resulting distribution is used to analyze the bonding characteristics. A cluster was modeled to simulated a based Fe alloy of 25% Cr-20% Ni type, with solid gamma structure [10], containing 99 atoms of iron, 45 atoms of Cr and 36 atoms of Ni distributed in five layers stacking (111) planes. The selected geometry for each plane is an equilateral triangle and the reference plane is the central one, which contains a vacancy. The calculations were performed using the ASED-MO (Atom Superposition and Electron Delocalization Molecular Orbital) method [11–14]. The modification of the Extended Hückel Molecular Orbital (EHMO) method was implemented with the YAeHMOP program [15].

The adiabatic total energy values were computed as the difference between the electronic energy (E) of the system when the H atom is at finite distance within the bulk and the same energy when that atom is far away from the solid surface. The "sequential hydrogen absorption energy" can be expressed as:

 $\Delta E_{\text{total}} = E(\text{FeCrNi} + H_n) - E(\text{FeCrNi} + H_{n-1}) - E(H)$ 

where *n* is the number of hydrogens, with n = 1 or 2.

The analysis of the theoretical results was made from the energy contour curves, covering all the (111) plane at steps of 0.05 Å. After determining the most stable position for the H atoms inside the  $Fe_{55}Cr_{25}Ni_{20}$  cluster, the electronic structure was computed. The change in the atomic orbital populations and the new chemical bondings were analyzed. To understand the interactions between the atoms, the concept of COOP (Crystal Orbital Overlap Population) curves was used. The COOP curve is a plot of the overlap population weighted DOS (Density Of States) vs. energy. The integration of the COOP curve up to the Fermi level ( $E_f$ ) gives the total overlap population of the bond specified and it is a measure of the bond strength.

## 3. Results and discussion

Under a sequential absorption scheme, up to two hydrogen atoms can be located in the Fe<sub>55</sub>Cr<sub>25</sub>Ni<sub>20</sub> cluster. The lower energy positions result to be the zone close to the vacancy (V). A schematic view of the H adsorption zone is presented in Fig. 1. The minimum V–H distances are 1.34 Å for H<sub>I</sub>, and 1.25 Å for H<sub>II</sub> locations. Fig. 2 shows the energy contour lines corresponding to the energy for the vacancy - two hydrogens (VH<sub>2</sub>) complex. We can see the H atoms aligned both along [1-10] direction and with the vacancy, in the (111) plane. This behavior can be related with the easiness of hydrogen trapping and, on the other hand, forming of a lineal hydrogen-vacancy clusterization, as a precursor to crack initiation. Tateyama et al. investigated the hydrogen effect on vacancy clusterization in BCC Fe [16]. VH<sub>2</sub> complexes are likely to favor line clusters along the (111) direction and also tabular one along  $\{110\}$  or {100} planes. The authors point out the implications of the hydrogen-enhanced vacancy activities in the H embrittlement phenomena. The {110} clusters are the first reasonable theoretical evidence of enhancement of fracture along these slip planes of BCC metals experimentally observed. In a previous study, we have showed that the VH<sub>4</sub> complex is likely to favor line clusters along the [-1 - 12] direction in the (111) plane of an FCC Fe–Ni alloy [17]. This repetitive pattern shows that hydrogen-vacancy clusterization may have a significant effect on the crack initiation.

Fig. 3(a) shows the DOS corresponding to the isolated  $Fe_{55}Cr_{25}Ni_{20}$  cluster. The alloy d states form a band starting at -14 eV and with a bandwidth of 8 eV while the s and p states are scattered and penetrating the d band. Fig. 3(b) shows the  $Fe_{55}Cr_{25}Ni_{20}$  cluster after the H atoms location. We can see the position of the H states after adsorption. The small contribution of H to DOS is due to its low concentration. A major view of H states can be seen in Fig. 3(c). The H projected DOS plot shows a deep Hs states located at lower energy values confirming the favorable hydrogen–vacancy interaction. The Fermi energy ( $E_f$ ) is -8.22 eV and it changes slightly with respect to the isolated cluster.

The H<sub>I</sub> (H<sub>II</sub>) atom are located near a Fe, Ni and Cr atoms at distances of 2.22 Å, 2.95 Å and 1.62 Å (2.28 Å, 2.78 Å and 1.56 Å), respectively. As consequence, the H–Fe, H–Ni and H–Cr interactions are formed. The H–Fe overlap populations (OP) are 0.082 (for H<sub>I</sub>–Fe<sub>I</sub>) and 0.053 (for H<sub>II</sub>–Fe<sub>II</sub>), while the H–Ni OP are 0.012 (for H<sub>I</sub>–Ni<sub>I,II</sub>) and 0.027 (for H<sub>II</sub>–Ni<sub>I,II</sub>), and finally, the H–Cr OP are 0.297 (for H<sub>I</sub>–Cr<sub>I</sub>) and 0.348 (for H<sub>II</sub>–Cr<sub>II</sub>), respectively (atom numbering references are shown in Fig. 1). The COOP curves for the H–metal interactions are showed in Fig. 4. As we can see, the H– metals are mainly bonding interactions and the biggest H–metal OP corresponds to the H–Cr interaction (H–Cr > H–Fe > H–Ni).

Hydrogen in the Fe<sub>55</sub>Cr<sub>25</sub>Ni<sub>20</sub> alloy due to affinities with the different metallic constituents induces local changes in bonding states. The atomic orbital occupations of the H nearest neighbor metallic atoms are modified after the H adsorption, these electron densities are summarized in Table 1. For the neighbor Fe atoms, the major changes are observed in Fe  $4p_x$  orbital whose population decreases to about 26% when the H is present. The contribution of Fe 4s population decreases to about 5% while the Fe  $4p_v$ ,  $4p_z$  and  $3d_{x^2-v^2}$  population diminishes between 2 and 4%. For the neighbor Cr atoms, the major changes are observed in Cr 4s,  $4p_v$ ,  $4p_z$  orbitals whose populations decrease to about 13%, and increase 39% and 18% respectively, when the H is adsorbed. The contribution of Cr  $3d_{x^2-y^2}$  population increases to about 11% while the Cr  $3d_{z^2}$  and  $3d_{xz}$ populations grow to about 7%. In the case of the Ni atom nearest neighbor to the hydrogen atoms, the Ni 4pz population decreases to about 7%. The contribution of the rest of Ni orbital population decreases less than 3%. The results indicate a majority participation of Cr and Fe orbitals in the hydrogens-alloy bonding. As predicted



Fig. 1. Schematic view of the H atoms location in the vacancy zone of the  $Fe_{55}Cr_{25}Ni_{20}$  alloy.

by the electronegativity differences, the Mulliken population analysis brings a partial negative charge on the H atoms while positive charge on the close neighbor Fe, Cr and Ni atoms, indicating an electron transfer to the H atom from the metallic nearest neighbor atoms. We observed the most important electron transfer corresponding to Fe nearest neighbor atoms. The electron transfer process helps to form the new H–metal bonds. As stated in previous paragraphs, hydrogen–vacancy clusterization occurs as



**Fig. 3.** (a) Total DOS for isolated  $F_{25}Cr_{25}Ni_{20}$  cluster, (b) total DOS for  $F_{25}Cr_{25}Ni_{20}$ -H-H cluster and (c) projected DOS for the H atoms in the  $F_{25}Cr_{25}Ni_{20}$ -H-H cluster.

a precursor to crack initiation. According, the H-metal reactions may take place in the domain of a crack tip and hence act as a fundamental component in initiating the SCC process.

The metallic bonds strength is modified after the H location. The Fe–Ni, Cr–Fe, Cr–Ni, Fe–Fe, Cr–Cr and Ni–Ni bonds nearest neighbors to the H atoms are affected, their OPs diminish 0.4%, 25%, 11%, 3%, 28% and 0.1%, respectively. As we can see, the nearest neighbor Cr–Cr, Cr–Fe and Cr–Ni bonds strengths are the most affected after H location. Fig. 5 shows the Cr–metal interactions, before and after H adsorption. We observe an OP diminish that is associated with the metallic bond weakening. The embrittlement mechanism helps to form the bonds between metals and H atoms and finally break the metal–metal bonds. This process plays an important role in subsequent localized corrosion nucleation.

In the present study, we can conclude that Cr atoms have an important role in the H-metal interactions because of the highest OP for H-Cr interaction and, on the other hand, the Cr-metals bonds strengths are the most affected after H adsorption. It was reported that the addition of hydrogen had a marked effect on the mechanical properties of the high Cr alloys [18]. Chromium may



Fig. 2. Contour lines corresponding to the energy (eV) for the  $Fe_{55}Cr_{25}Ni_{20}-H-H$  system at the vacancy (V) zone.



Fig. 4. COOP curves for H-metal interactions in the Fe<sub>55</sub>Cr<sub>25</sub>Ni<sub>20</sub>-H-H cluster.

#### Table 1

Orbital occupations for the atoms whose participate in the interactions.

| Atom               | S                   | p <sub>x</sub> | p <sub>y</sub> | pz     | $d_{x^2-y^2}$ | d <sub>z<sup>2</sup></sub> | d <sub>xy</sub> | d <sub>xz</sub> | d <sub>yz</sub>     |
|--------------------|---------------------|----------------|----------------|--------|---------------|----------------------------|-----------------|-----------------|---------------------|
| HI                 | 1.3588 <sup>a</sup> |                |                |        |               |                            |                 |                 |                     |
| HII                | 1.3627 <sup>a</sup> |                |                |        |               |                            |                 |                 |                     |
| Fe <sub>I</sub>    | 0.6565              | 0.0595         | 0.0766         | 0.0748 | 1.3054        | 1.3261                     | 1.4035          | 1.3187          | 1.2532 <sup>a</sup> |
|                    | 0.6922              | 0.0808         | 0.0779         | 0.0765 | 1.3659        | 1.3390                     | 1.3952          | 1.3464          | 1.2655 <sup>b</sup> |
| Fe <sub>II</sub>   | 0.6614              | 0.0633         | 0.0732         | 0.0798 | 1.3482        | 1.3264                     | 1.3933          | 1.3640          | 1.2739 <sup>a</sup> |
|                    | 0.6972              | 0.0856         | 0.0749         | 0.0823 | 1.3869        | 1.3416                     | 1.3838          | 1.3617          | 1.2815 <sup>b</sup> |
| Cr <sub>I</sub>    | 0.5090              | 0.0668         | 0.0534         | 0.0753 | 0.5410        | 0.6829                     | 0.6916          | 0.5959          | 0.5633 <sup>a</sup> |
|                    | 0.5784              | 0.0662         | 0.0520         | 0.0637 | 0.5448        | 0.7271                     | 0.6919          | 0.5576          | 0.5448 <sup>b</sup> |
| Cr <sub>II</sub>   | 0.4986              | 0.0602         | 0.0739         | 0.0496 | 0.5551        | 0.6639                     | 0.7199          | 0.5331          | 0.4987 <sup>a</sup> |
|                    | 0.5739              | 0.0600         | 0.0530         | 0.0453 | 0.4969        | 0.6595                     | 0.7235          | 0.5355          | 0.5256 <sup>b</sup> |
| Ni <sub>I,II</sub> | 0.9465              | 0.3757         | 0.3726         | 0.3503 | 1.8834        | 1.8780                     | 1.8912          | 1.9253          | 1.9224 <sup>a</sup> |
|                    | 0.9621              | 0.3795         | 0.3822         | 0.3764 | 1.8836        | 1.8747                     | 1.8878          | 1.9257          | 1.9197 <sup>b</sup> |

<sup>a</sup> After H atoms location.

<sup>b</sup> Before H atoms location.

have two effects: 1) it may increase the strain required to initiate voids; and 2) it may increase the strain required for the voids to coalesce. Since the failure strain is much higher in the high-Cr alloys, it appears that microvoid nucleation and/or growth processes occur at higher strains with increasing chromium content. A maximum in embrittlement was observed in upper 25% Cr allow where the elongation to failure was reduced from 53% to 14%. Other effect of alloving elements is to alter the stacking-fault energy, which in turn affects the mode of deformation. The loss in ductility appears to be inversely related to stacking-fault energy. A maximum in embrittlement was observed in the 26% Cr alloy and it was coincided with the minimum in stacking-fault energy [19,20]. On the other hand, if either a decohesion mechanism or a void nucleation mechanism is important, then the yield strength would be important [21,22]. An increase in the yield stress will increase the local stress at a particle and allow decohesion to occur at a lower strain. This is consistent with the change in strain-



**Fig. 5.** COOP curves for Cr–Cr interaction, (a) before and (d) after H adsorption. COOP curves for Cr–Fe interaction, (b) before and (e) after H adsorption. COOP curves for Cr–Ni interaction, (c) before and (f) after H adsorption.

hardening behavior observed in these alloys as a function of chromium concentration [18]. Increasing the chromium content of the alloy increased the solubility of hydrogen at chromium contents greater than 15%. Tests that were analyzed to determine the percent reduction in area of the 6% Cr and 15% Cr alloys with the same hydrogen concentration, showed that the 15% Cr alloy was embrittled more [18].

Hydrogen embrittlement effects can take the form of ease of crack initiation and/or propagation or the development of hydrogen-induced damage, such as surface blisters and cracks or internal voids [23]. It appears that any material can become embrittled by a pressure effect if hydrogen bubbles are introduced and this state remains unchanged until hydrogen atoms escape from the bubbles [24]. In the present study, some H–H association is present in the Fe<sub>55</sub>Cr<sub>25</sub>Ni<sub>20</sub> cluster. The COOP curve corresponding to the H-H interactions is shown in Fig. 6. This curve presents bonding and antibonding peaks below Ef. The integration up to the Fermi level gives a total OP for the H–H bonding in the cluster. We can confirm that at the H–H distance of 2.59 Å, a H–H interaction with an OP value of 0.004 is formed. According to the literature, a typical H<sub>2</sub> chemical bond is formed at the interatomic distance of 0.74 Å. By ASED calculation, in the vacuum, the H-H OP at the distance of 0.74 Å is 0.15. As we can see, the H–H distance in the Fe<sub>55</sub>Cr<sub>25</sub>Ni<sub>20</sub> cluster is bigger and the H–H OP is smaller, than the corresponding for the H<sub>2</sub> molecule in the vacuum. Then, the



Fig. 6. COOP curves for the H–H interaction in the Fe<sub>55</sub>Cr<sub>25</sub>Ni<sub>20</sub>–H–H cluster.

formation of a typical hydrogen bond is not evident in the  $Fe_{55}Cr_{25}Ni_{20}$  cluster.

# 4. Conclusions

The theoretical calculations contribute to interpret the changes in the  $Fe_{55}Cr_{25}Ni_{20}$  electronic structure and the chemical bonding after the H adsorption to better understanding the H embrittlent phenomenon by decohesion mechanism of iron–chromium– nickel alloys.

The H atoms are trapped in the zone of the  $\gamma$ -Fe<sub>55</sub>Cr<sub>25</sub>Ni<sub>20</sub> vacancy. The impurities are located aligned both along [1–10] direction and with the vacancy, in the (111) plane. This behavior can be related with the easiness of hydrogen trapping and forming a lineal hydrogen–vacancy clusterization, as a precursor to crack initiation.

An electron transfer to the H atoms from the Fe, Cr and Ni nearest neighbor atoms is observed. The electron transfer process helps to form the new H–metal bonds. The atomic orbital occupations of the metallic bonds close to the H atoms are affected. The mainly changes are presented in Cr  $4p_y$  and Fe  $4p_x$  orbitals. The  $3d_{x^2-y^2}$ ,  $3d_{z^2}$  and  $3d_{xz}$  metallic orbitals have also participation in the hydrogens–metal interactions.

The strengths of the metallic bonds nearest neighbors to the H atoms decrease. The Cr atoms have an important role in the embrittlent process, the H–Cr OP is the highest and the Cr–metals bonds strengths are the most affected after H adsorption.

We found same H–H interaction that could be associated with the precursor of hydrogen bubble but it is far away to a typical  $H_2$  chemical bond.

The embrittlement mechanism helps to form the bonds between metals and H atoms and finally break the metal—metal bonds. These processes play a key role in subsequent localized corrosion nucleation such as the initiation of stress corrosion cracking.

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