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Chemostructural Conditionalities for Welderbility in Nickel-Chromium Sequenced Dual Nucleation

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Abstract*: -** The structural conditions required to form and sustain a weld is dependent on the dynamics of chemical combinations using heat as a catalyst in some instances and weld types. The relevant combinatorial for this to happen in the Nickel-Chromium complex have been considered and results have shown that internuclear forces are principally critical in order to sustain the chemostructural equilibrium required to maintain a weld. Thus, a weld is degraded in value and strength when, due to a rise in temperature, this balance is compromised and the valence space factor ***μ is *depotentiated above its existential ambivalence*. Consequently, welderbility conditions require that the chemical compositions of a weld remain within the limits of allowable tolerance.

I.   INTRODUCTION

Chemostructural conditionalities in relation to welding and weldability results from the fact that welding revolves around the practice of chemical reactions and bonding between constituent metallic elements or alloys at elevated temperatures; while subjecting the entire process to predetermined conditions that are structurally supportive to the intendment of the design. The foregoing implies that an understanding of the reactivity or chemical combinations of these constituent elements is principally critical to a better application of fusion welding. Thus, chemostructural conditionalities with respect to this paper refers to the intrinsic values and characteristics required for the reversible equilibrium of reacting elemental combinations, that are dependent on temperature rise and the fluidized properties of metals and their alloys.

As the study would reveal, the essence of temperature in welding conditions borders on the thermochemical requirements for dislocation of intermolecular binding energies; which upon achievement is a very instrumental conditionality in terms of reactivity with other elements.

The study shall consider the relative nature of these reactions that are dependent on temperature rise and how this requirement enhances the manufacture of engineering materials with multi-attribute capabilities and characteristics-being contributory framework of their constituent components. This study is about the nature of the bonding of these metals in conditions of temperature rise and how this bonding results metallic fluids with varying fluidity indices that are relatively relevant to various engineering applications.

II.   NATURE OF THERMOCHEMICAL BONDS IN WELDING PROCESSES

It has been stated that thermochemical bonds are complementary results of fusion energies observed during high temperature activities where metals bond with each other, based on specific conditions such as the Hume-Rothery Rule on chemical bonding in the case of *substitutional solid solutions* [1]. Thus, the rule requires that:
(i) the two metals must be of similar crystal structures and,
(ii) the difference in their atomic radii should be less than 15%.

It should be emphasized that this solute-solvent relationship also extend to *interstitial solid solutions* where the size of the solute atom is much smaller than that of the solvent atom, thus enabling the solute atoms to occupy interstitial positions. Consequently, two conditions apply, namely:
(i) the solvent atom must have more than one valence
(ii) the atomic radius of the solute must be less than 59% of the atomic radius of the atom.

In view of the foregoing, these rules guide the bonding requirements for alloys as in the case of steel where carbon atoms occupy interstitial positions between iron atoms in the sizes that are compliant with the stated rules. This is illustrated in the FeC combination, where the atomic radius of carbon is 0.071nm, that of iron atom is 0.124nm radius; the radius of carbon being less than 59% radius of iron. Considering this fact of chemical bonding and reactivity, it is safe to posit that, beside these identified *solid fluids*, there exist another group of solid fluids that are alloys in nature and they are referred to as *intermetalic compounds* and their type of bonds may range from metallic to ironic. Thus, weld electrodes and fluxes fall within these materials.

Further, these intermetallic compounds consist of electrons arrayed between cations such that internuclear forces of attraction of individual atoms exerts forces on these electrons based on affinity considerations resulting from their electropositivity relativities and thus binds them to one another in sequential and symmetrical dimensions that they impart and retain their structures. This determines the various properties associated with such materials.

Consequent on these rules, these chemical combinations are only made possible because the metal elements posses bonding orbitals that responds to the *Pauli exclusivity* correlations which asserts that, 'no more than two electrons may occupy any orbital and if two do occupy it, their spin directions must be opposed'. [2] In the line of this argument, a careful study of the *Aufbau principle* [2] draw attention to the fact that even though the *Pauli exclusivity principle* has made a categorical statement, the bonding of multiple atoms only distort the orbital resolutions which has no direct consequence to the exerting force of the nucleus on the electrons aligning the orbitals. Thus, the more contribution of electrons from individual atoms, the more the exerting pulls of the nucleus of all the atoms on all the electrons in the shared and distorted orbitals. This valence bond theory can be illustrated in the thermochemical bonding arrangement of stainless steel type 330; where composition is as follows: Ni-36%, Cr – 16%, Fe-52% [3]. The chemostructural conditions supporting this stainless steel material is as follows:
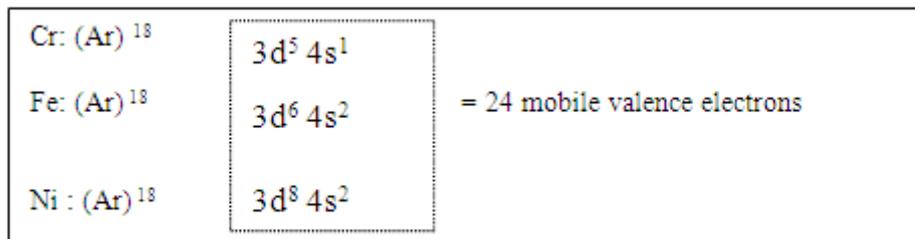

Figure 1: Valence bonding electrons

A proper view of Fig. 1 would indicate that, the *Ligand Field Theory* would be more appropriate explanation in determining the combinatorial dynamics of the complex bonding and symmetrics resulting electrostatic and cris-crossing overlapping interactions that are characteristic of molecular orientations in metallic conditions. This implies that the strength of any bond depends on the degree to which the orbitals overlap each other. Relatively, for the Ni-Fe-Cr structure, the molecular overlap can be defined as:

$$S = \int \psi_A(r)\, \psi_B(r)\, \psi_C(r) d\tau \,\ldots\ldots\ldots\ldots\, (1)$$

Thus, this equation resolves the aggregate interdependences of the *thermochemical force vectors* and their energy components in the Ni-Fe-Cr lattice. Further, a careful observation of Fig. 1 reveals that all the reacting metals belong to the transition *d-orbital* group of metals, implying that their strength lies in the binding energies contained in their *d-orbitals*. Further, a total of 24 valence electrons are noticed to constitute an *electron cloud* and pictorially could be viewed as follows:
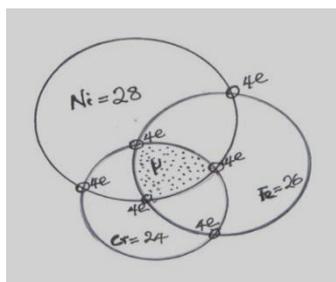

Figure 2: Molecular Overlap for Ni-Fe-Cr complex

It should be noted that the valence electron located at the *d and s* overlap, maintains a tetrahedral shape as in Fig. 2 above. The electron cloud of 24 *d and s* electrons are found to be arranged into four electrons (i.e. 4e) for every point of orbital overlap in the tetrahedral structure. It could be seen that these points of overlap are 6 in number representing 24 electrons. Atkins [2] observed that in a tetrahedral structure of this nature, some point of overlap are identifiable, having both positive and negative poles which this study observe, enables axial orientation during mobility and bonding. Further, it could also be noticed that while there are internal bonding due to the overlap of orbitals, there is also evidence of external bonding giving rise to a structure whose surface tensions are protective to the internal bonding. Thus, it would require a higher secondary external influence to depotentiate this internal bond. The paper views this constraint as a proclivity towards *dual nucleation*.

In view of the findings of this study, mobility and bonding are occasioned by temperature rise and chemical reactions. This paper therefore is of the view that, if the doted energy zone in Fig. 2 is geometrically analyzed, the area of a triangle enclosed by the overlap of the individual atoms is a unity, or an approximated unity within a bounded region $S \leq 1$ or $S \geq 1$. It should therefore be noted that the length of the sides of this triangle is dependent on the bond length of the constituent elements. This forms the basis for the approximation in the area of the triangle enclosed by the *valence space factor*, **μ**. Thus;

$$S = \int \psi_A(r) \ \psi_B(r) \ \psi_C(r)d\tau \geq 1 \dots\dots\dots\dots\dots\dots(2)$$

The implication of Fig. 2 and its derivative equation (2) is that while the individual atoms in the combination exert nuclear forces of attraction on their valence electrons to maintain the required shape and strength, a defined zone, **μ** (referred to as the valence space factor) exist where standard equilibrium conditions resulting the stability of the metal is guaranteed. Thus, **μ** is the highest point of stability and strength, since it constitute a zone where *contributory strength* is in the order of (10:8:6)e; and definitive of the structural requirements of stainless type steel 330. Hence, the bonding conditions in this reaction results the following properties of this alloy [3]:

Table 1: Weldability Properties of Stainless steel type 330 (Ni-Fe-Cr)

Material	Nominal Composition (essential elements)	Yield strength 1000lb./sq.in	Tensile strength 1000lb./sq.in	Hardness, Brinell	Density, lb/cu.in	Specific gravity	Melting point,°F	Specific heat, B.t.u/(lb) (°F)	Thermal expvty. Coef.	Thermal cond. (sq.ft)(hr) (°F/in)
Stainless steel type 330	Ni 36,Cr 16, Fe bal	55	100 (hot) 80(annealed) 150 (cold)	200	0.284	7.86	2515	0.11	6.3 8.3	90

It should further be mentioned that the properties stated in Table 1 above enhances the weldability of stainless steel type 330 and as could be seen, the melting point of 2515°F implies an aggregate heating value necessary to cleave the Ni-Fe-Cr binding effects of the interposed bonds of Fig. 2 to the point where engaged molecular forces resulting **μ** are broken and associated bond energies are released to enhance further reactivity with other elements within the reactivity range of the alloy. Further, effect of temperature could be seen in the fact that while tensile strength of the cold drawn material is 150 lb/sq.in, that of hot drawn is 100 lb/sq.in, implying that the binding energies in the bonds and most especially within the *valence space factor μ*, are broken to achieve the new structure after reaction.

III.   DISCUSSIONS :BASE – FILLER COORDINATION IN WELDING CONDITIONS

Base-filler coordination has to do with molecular interactions between base metals or alloys and filler metals or alloys. Thus, the strength of welded joints depends on these thermochemical conditions. As could be seen in Table 1 above, 2,515°F of temperature is required to melt the Ni- Fe-Cr- alloy. This fluidity condition entails the use of heat from elevated temperatures to break metallic bonds and thus, occasion the release of the energies stored in those bonds. When this is achieved, atomic combinations between molecules become possible. In view of this possibility, it should be noted that nickel and nickel based alloys do not require pre-heating; but base metal temperature should be raised to 16°C or more to avoid moisture condensates that could result porosity at the weld joint [4].

In furtherance of the foregoing position, it is imperative to state that, filler metals do not have the same melting point as the base metals. This implies that, at the melting point of the filler metal, the base metal structure has been affected by the same heat and metallic bonds (of the base metals) at that point have been made weaker or broken. This thermodynamic condition is very critical to bond formation during welding. Thus,

if the orbital overlap in Fig. 2 above represent a welding point that has been affected by weld temperature (HAZ) and the filler metal is nickel based alloy or metal, valence electrons of the filler material thus proceeds to attach itself to the Nickel atom of the base material, and also attach itself to the other non-nickel atoms of the base material by donating its valence electrons to be shared in the coordination.

The bonding forces from these orbitals still utilize the *d-orbital* as discussed previously. As Table 2 below indicates, while the melting point of Cr is 1857^oC that of Fe is 1537^oC and Ni is 1455^oC, it would be more appropriate to use Nickel metal or alloy for the filler metal. This is because the melting point of the stainless steel type 330 Ni-Fe-Cr is 2515^oF.

Table 2: Constituent bonding and reactivity properties of Ni- Fe-Cr- alloy

Element	Cr	Fe	Ni
Electron Configuration	$3d^5 4s^1$	$3d^6 4s^2$	$3d^8 4s^2$
First Ionization energy (kJ/mol)	653	759	737
Bonding Atomic Radius (A)	1.27	1.25	1.21
Density (g/cm^3)	7.9	7.9	8.9
Melting Point (^oC)	1857	1537	1084

However, in an experiment to determine percentage availability of ferrite and austenite in the welded joint of Ni based alloy, it was suggested [4] that filler metals should be carefully selected to fall within the range of the base metal. This implies that temperature range should not be too far apart as to enhance chemical bonding between the orbitals of the combining or reacting metals. Regard therefore should be made to ensure that *thermal diffusibility* does not abolish the joint in the sense that a particular metal can completely diffuse in another as the case where Tin is the filler metal and Titanium is the base metal during temperature rise condition [1]. Studies have also reinforced the position that filler metals should be close ranged on base metals to achieve better results as this improved the *acicular ferritic conditions* (AFC) of the weld, [5,1] thus increasing its mechanical properties as indicated in the Fig. 4 and Fig. 5 below :
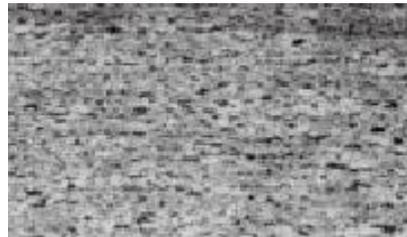
Figure 4 Weld structure *without* N_1 filler on Ni base

Figure 5 Weld structure *with* Ni filler on Ni base

From Fig. 5 above, the coarse fracture surface indicate additional bonding characteristics mainly due to Ni interactions as has been explained previously.

IV.   CONCLUSION

As have been stated, the relevance of the *d-orbital* in the determination of bond strength indicates the application of both valence bond theory and the ligand band complexes. The interplay resulting from the overlapping is very critical to the bond strength which directly defines the strength of the welded joint. It is therefore instructive to mention, that temperature play a key role in this development, since it is the means of making the orbital respond to external combinatorials, especially where the base metal is chemically compatible with the filler metal as have been seen in Fig. 5 above. Thus, bond strength has to do with the individual nucleus

potentials of the ligands or complexes; for which an attractive pull exerted on the electrons creates stability and equilibrium which by extension influences the entire strength of the weld.

Thus, the value of μ in Fig. 2 has direct consequence on the strength of the weld joint, which can be determined by various impact and NDT assessment. The study finds that the failure of μ is the failure of the welded joint. However, it should be noted that beside the critical relevance of μ, other factors also enhances joint strength, such as temperature, hydrogen presence, defective fluxing, etc. Though, all these constitute physical conditions for welderbility, the microstructural and chemostructural relativities are more critical as they addresses the molecular origin of the bonds and thus influences the bonding parameters and structural mechanics of the possible chemical combinations during welding and other heat treatment conditions required for orbitals to bond.

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