First-principle calculation of stainless steel 304N used in concrete-filled steel tubular

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Abstract: stainless steel 304N was calculated in the paper for the possible use in concrete-filled steel tubular. Calculation results show that compared with conventional 304 ferrite stainless steel, 304N adds alloy element niobium. Because Nb has strong effect of fixing carbon and nitrogen and refining ferrite grain size, 304N has very uniform and fine ferrite structure in annealing state, and carbonitride precipitates very little at grain boundary. Its corrosion resistance, formability, weldability and wrinkle resistance are better than ordinary 304.

1. Introduction
Ferritic stainless steel is a kind of stainless steel containing 10-30% chromium. Common 304 have three shortcomings [1-3]. First, it has poor corrosion resistance and is prone to intergranular corrosion. Secondly, the weldability is general [4]. There is a certain gap between the performance of the weld and the base metal after welding. Thirdly, the forming performance is insufficient, which shows that it is easy to crack after deformation [5]. To deal with such shortcomings, Nb-containing ferrite stainless steel was present and calculated in the paper.

2. Calculation method
Thermodynamic stability of Nb (C,N) was calculated first. Then, Comparison of diffusion activation energies of Nb(C,N) and C,N. Simulations were performed using the density functional theory based CASTEP 2018 code. Ultra-soft pseudo potentials with cut-off energy of 500 eV were used throughout. The Perdew, Burke and Emzerhof parametrisation of the generalised gradient approximation was employed to describe the exchange correlation function. A Monkhorst-Pack sampling scheme was used for the integration of the Brillouin Zone, with a minimum k-point separation of 0.045 Å⁻¹. The simulations employed density mixing using the Pulay method. The energy convergence criterion for self-consistent calculations was set to 1 × 10⁻⁸ eV and the maximum allowed forces between ions was 1 × 10⁻² eV/Å.
All simulations were performed until a maximum difference in energy of $1 \times 10^{-5}$ eV and atomic displacement of $5 \times 10^{-4}$ Å between iterations was achieved. Non-defective structures were relaxed under constant pressure to the above convergence criteria.

DMol3 calculations are Local density approximation based on finite temperature (with free energy as a variable). The instantaneous electron ground state is solved for each MD step with a valid matrix diagonal scheme and an effective pulse. These techniques can avoid all the problems that are present in the original Car-Parrinello method. The interaction of ions and electrons is described by the FLAG or the projection extended wave (PAW) method. Both techniques can considerably reduce the number of plane waves necessary for each atom of the transition metal or first row element. The truncation of the plus projection wave can be 12.25Ry.

3. Calculation results and discussion

3.1 (P–B) ratio of Nb
The (P–B) ratio of each metal ion in the oxide film is formed by the combination of metal and oxygen to the volume of each metal atom in the metal. It reflects the stress state in the oxide film. Compared with the metal between 1~ 2, the surface oxide film produces a certain degree of compressive stress, the film is dense, and the metal oxidation resistance is strong. When the P–B ratio is less than 1 or more than 2, the tensile stress or excessive compressive stress is produced in the oxide film, which is easy to cause the film to break and the metal oxidation resistance is low.

Calculation results in Castep show P–B ratio of Nb is 1.438. as seen $1 < R_{PB} < 2$: the oxide coating is passivating and retard further surface oxidation[6].

3.2 Binding energy of some compounds
Binding energy refers to the energy released by the combination of two or more particles into larger particles, or the corresponding particles to decompose into the energy to be absorbed by the original particles. These two expressions are equivalent.

In nuclear physics, binding energy is the energy one needs to break the nuclear force and to separate the nucleus into individual protons and neutrons. In the other words, the binding energy represent the difference between the masses of the nucleus and the sum of the individual masses of the nucleons.

| compounds | NbC   | NbN   | FeC   | FeN   | CrC   | CrN   |
|-----------|-------|-------|-------|-------|-------|-------|
| $\Delta G_f^0$ | -0.26870 | -0.35634 | -0.1437 | -0.08087 | -0.2137 | -0.15133 |

As seen as table 1, Whether carbon or nitrogen atoms, it is easier to combine with niobium atoms to form more stable compounds, so carbon is not easy to react with chromium to cause so-called chromium depletion[7].

3.3 Diffusion activation energy of some substances in alpha-ferrite
The diffusion pathways and activation energies that govern atomic transport within ferric materials control the rate at which corrosion can be formatted. Such calculation was done in CASTEP.

| substances | C | N | NbC | NbN |
|-----------|---|---|-----|-----|
| activation energies | 85 | 56 | 345 | 297 |

As seen as table 1, the diffusion activation energies of NbC and NbN are very large, which makes it difficult for carbon and nitrogen to leave the cell and enter the grain boundary, and combine with chromium, resulting in the decline of corrosion resistance[8].
4. conclusions
We can safely draw conclusions as follows.

1) According to P-B ratio, Nb is not bad for anticorrosion of ferric materials.
2) Nb(C, N) is much stable than Fe(C, N) or Cr(C, N), and Nb(C, N) is much more difficult leaving from the alpha-ferric lattice. Both of them improve the anticorrosion of ferric materials.

Acknowledges
This work was supported by the Scientific and Technological Research Program of Chongqing Education Commission (KJ1503305), State Key Laboratory of Complex Nonferrous Metal Resources Clean Utilization / Kunming University of Science and Technology (CNMRCUKF1603), Chongqing Vocational Institute of Engineering (JG182022).

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