First-principle and molecular dynamic calculation of concrete-filled steel tubular to introduce stainless steel technology

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Abstract: The concrete-filled steel tubular (CFST) structure offers numerous structural benefits, including high strength and fire resistances, favorable ductility and large energy absorption capacities. There is also no need for the use of shuttering during concrete construction; hence, the construction cost and time are reduced. These advantages have been widely exploited and have led to the extensive use of concrete-filled tubular structures in civil engineering structures. In the existing dozens of species types of stainless steel, some are suitable for concrete-filled steel tubular, some not. In this paper, the principles for selection of such types are studied, by both quantum mechanism and molecular dynamic method.

1. Introduction

In metallurgy, stainless steel, also known as inox steel or inox from French inoxydable (inoxidizable), is a steel alloy, with a minimum of 10.5% chromium content by mass and a maximum of 1.2% carbon by mass.

Concrete-filled stainless steel tubular (CFSST) columns are increasingly used in modern composite construction due to their high strength, high ductility, high corrosion resistance, high durability and aesthetics and ease of maintenance.

In the existing dozens of species types of stainless steel, some are suitable for concrete-filled steel tubular, some not. In this paper, the principles for selection of such types are studied, by both quantum mechanism and molecular dynamic method.

2. Calculation method

On the basis of the P–B ratio, it can be judged if the metal is likely to passivate in dry air by creation of a protective oxide layer. P–B ratio simulation was done with CASTEP 2018, a very good code using...
quantum theory, using ultra-soft pseudo potentials with a cut-off energy of 380 eV. The Perdew, Burke and Ernzerhof 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.

In calculation, the most factors include the self-consistent energy convergence criterion, the maximum allowed forces between ions, maximum difference in energy, and atomic displacement. They were set to $1 \times 10^{-8}$ eV and $1 \times 10^{-2}$ eV/Å, $1 \times 10^{-5}$ eV and $5 \times 10^{-4}$, respectively. Finally, it resulted in a 36 atom supercell.

Melting point of metals and their oxide was calculated by LAMMPS, a very good simulation code using potential filed model including der Waals and electrostatic interactions. A time step, coupling constant, cutoff, and accuracy are 4 fs, 0.4 ps, 12.0Å, of $10^{-4}$, respectively. NVT ensemble was adopted using the leap-frog algorithm with a time step of 2.5 fs. annealed time and gather time of the structures of metal and their oxides were set to 30 ps and 320 ps.

3. Calculation results and discussion

3.1. PBR values

PBR values of 1~2 is most important condition for stainless steel\cite{4,5}

| PBR value of metals | PBR value |
|---------------------|-----------|
| brand No. (USA)     |           |
| 302                 | 2.075     |
| 303                 | 2.081     |
| 304                 | 2.087     |
| 304L                | 2.083     |
| 309S                | 2.088     |
| 310S                | 2.088     |
| 316                 | 2.289     |
| 316N                | 2.187     |
| 316L                | 2.283     |
| 405                 | 2.088     |
| 430                 | 2.092     |
| 430F                | 2.092     |
| 403                 | 2.095     |
| 410S                | 2.096     |
| 410                 | 2.095     |
| 420                 | 2.089     |
| 420                 | 2.161     |
| 201                 | 2.091     |
| 202                 | 2.092     |

As seen from table 1, 316L is higher than others, maybe caused by Mo, an element with high PBR value.

Quantum mechanism calculations results show that 316L is not suitable in preventing corrosion and conform. The table also shows that the corrosion inhibition of these compounds is the same. We can safely draw a conclusion that most metals are fit to inhibit by the PRB value.

3.2. melting points

High melting points is very important factor for concrete-filled steel tubular\cite{6,7}.
Table 2 melting points of metal oxides

| brand No. (USA) | melting points |
|-----------------|----------------|
| 1Cr18Ni9        | 302            | 1421          |
| Y1Cr18Ni9       | 303            | 1435          |
| 0Cr18Ni9        | 304            | 1427          |
| 00Cr18Ni9       | 304L           | 1424          |
| 0Cr23Ni13       | 309S           | 1429          |
| 0Cr25Ni20       | 310S           | 1432          |
| 0Cr17Ni12Mo2    | 316            | 1442          |
| 0Cr17Ni12Mo2N   | 316N           | 1275          |
| 00Cr17Ni14Mo2   | 316L           | 1444          |
| 0Cr13Al         | 405            | 1396          |
| 1Cr17           | 430            | 1435          |
| Y1Cr17          | 430F           | 1437          |
| 1Cr12           | 403            | 1437          |
| 0Cr13           | 410S           | 1438          |
| 1Cr13           | 410            | 1437          |
| 2Cr13           | 420            | 1437          |
| 3Cr13           | 420            | 1437          |
| 1Cr17Mn6Ni5N    | 201            | 1134          |
| 1Cr18Mn8Ni5N    | 202            | 1133          |

As seen from table 1, 201,202L are much lower than others, maybe caused by N, a element with low melting points[8].

Molecular dynamic calculations results predict that 316L is not suitable in preventing corrosion because their melting point is low.

4. Conclusions
The relationship between the intrinsic properties and the deformation behavior of the material was describing for measuring the intrinsic energy barriers. From such discussion, conclusions can be drawn safely that series 2** and 316L is not suitable to concrete-filled steel tubular.

The paper opens up a new way to investigate and understand materials from a different perspective. Much practical work was requiring proving the conclusions.

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