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# Elastic Properties of $FeCr_{20}Ni_8X_n$ (X = Mo, Nb, Ta, Ti, V, W and Zr) Austenitic Stainless Steels: A First Principles Study

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**Abstract:** Austenitic stainless steels suffer from intergranular corrosion and stress corrosion cracking when exposed to elevated temperature (500–800 °C). Under these environments, Cr-carbides and Cr-carbontrides precipitate at the grain boundaries, which results in the formation of Cr-depleted zone. In practice, alloying elements could be added into austenitic stainless steels to modify the precipitation processes. Besides the precipitation processes, the elastic properties of the iron matrix would be influenced. Using the exact muffin-tin orbitals (EMTO) method, the solute effects on the elastic properties of FeCr<sub>20</sub>Ni<sub>8</sub> austenitic stainless steels were studied. Based on the simulated shear modulus (*G*) and bulk modulus (*B*), we proposed a design map for FeCr<sub>20</sub>Ni<sub>8</sub> based alloys, aiming to provide a basis for the design of high-performance austenitic stainless steels.

Keywords: stainless steels; elastic properties; first principles; solute effects

# 1. Introduction

Austenitic stainless steels are widely used in the nuclear, oil and chemical industries, owing to their excellent mechanical properties, weldability and corrosion-resistance properties [1–4]. However, when exposed to elevated temperature (500–800 °C), these alloys become susceptible to intergranular corrosion and stress-corrosion cracking. Under these environments, Cr-carbides and Cr-carbontrides precipitate at the grain boundaries, which results in the formation of the Cr-depleted zone [5–7]. To overcome this drawback, strong carbide-forming elements are added to reduce the concentration of C, aiming to suppress the Cr-carbides and Cr-carbontrides and avoid the formation of Cr-depleted zone [3,8,9]. It should be noted the addition of carbide-forming elements not only influences the precipitation processes, but also changes the elastic properties of the iron matrix.

Using ab initio simulations, Vitos et al. investigated the elastic properties of the  $Fe_{100-(c+n)}Cr_cNi_n$  alloys (13.5 < c < 25.5 and 8 < n < 24) [10,11] (here and throughout the paper, the concentrations are expressed in the atomic percentage, at.%). In that work, shear modulus (*G*) and bulk modulus (*B*) fall into the range of 74–81 GPa and 161–178 GPa, respectively. These authors revealed a very interesting trend that relatively high values of *G* correspond to relatively low values of *B*, and vice versa. For example, FeCr<sub>20</sub>Ni<sub>8</sub> (corresponding approximately to alloy steel AISI 304) has an intermediate value of *G* (77.3 GPa) but a low value of *B* (165.2 GPa) [10].



It should be noted that a lower value of *B* means the atomic bond is weaker. Consequently, materials with a low value of *B* exhibit relatively poor resistance to various forms of localized corrosion (such as intergranular corrosion, pitting corrosion and stress-corrosion cracking) [10,12–14]. Furthermore, Clerc et al. have demonstrated the hardness of the annealed metal is proportional to *G* [15]. It is commonly known that high a value of the B/G ratio (>1.75) often results in ductility, while a low value of the B/G ratio (<1.75) often results in brittleness [10,11,14,16–18].

Potentially, alloying elements (such as Mo, Nb, Ta, Ti, V, W and Zr) might be added into austenitic stainless steels to suppress the Cr-carbides and Cr-carbontrides. In addition to the precipitation processes, the elastic properties of the iron matrix would also be influenced. In this work, we simulated the solute effects on the elastic properties of FeCr<sub>20</sub>Ni<sub>8</sub> austenitic stainless steels. We also calculated the difference ( $E_{BCC}-E_{FCC}$ ) between body-centered cubic (BCC) and face-centered cubic (FCC) structure. The solute concentrations considered in this work are 1 at.% and 2 at.%.

### 2. Computational Methods

In this work, all calculations were calculated at 0 Kelvin. We performed first principle simulations based on the exact muffin-tin orbitals (EMTO) method [19,20]. The coherent potential approximation (CPA) was used to describe the random alloys [21,22]. A  $29 \times 29 \times 29$  k-point grid was used to sample the Brillouin zone. In self-consistent calculations, the total energy converged within  $10^{-7}$  Ry per atom. Frozen core approximation, disordered local magnetic moment (DLM) [23], and the local density approximation (LDA) [24] were adopted to calculate the charge density. Then, the total energy was evaluated with the full charge density technique (FCD) approach [25]. In the FCD calculation, the exchange–correlation interactions were described by the generalized gradient approximation (GGA) in the Perdew–Burke–Ernzerhof (PBE) form [26]. This combination of approximations has been used to calculate the equation of state of Fe–Cr–Ni alloys successfully [10,16]. Using EMTO package 5.8, provided by Professor Levente Vitos (Royal Institute of Technology, Stockholm, Sweden) [20], we calculated the total energies of various distorted unit cells. The bulk modulus *B* is obtained by fitting the total energies as a function of the unit cell volume [27,28].

$$E(V) = E(V_0) + \frac{B_0 V}{B'_0} \left(\frac{(V_0 / V)^{B'_0}}{B'_0 - 1} + 1\right) - \frac{B_0 V_0}{B'_0 - 1}$$
(1)

where E(V) is the energy for individual V;  $E(V_0)$  is the energy at the equilibrium unit cell volume  $V_0$ ;  $B_0$ , and  $B'_0$  are the bulk modulus and its pressure derivative at  $V_0$ .

To calculate the tetragonal shear modulus C', an orthorhombic distortion is applied to the unit cell.

$$I + \varepsilon = \begin{pmatrix} 1 + \delta & 0 & 0 \\ 0 & 1 - \delta & 0 \\ 0 & 0 & \frac{1}{1 - \delta^2} \end{pmatrix}$$
(2)

Then the tetragonal shear modulus C' is fitted as the following:

$$\Delta E(V) = 2VC'\delta^2 + O\left[\delta^4\right] \tag{3}$$

To calculate the  $C_{44}$ , a monoclinic distortion is applied to the unit cell.

$$I + \varepsilon = \begin{pmatrix} 1 & \delta & 0 \\ \delta & 1 & 0 \\ 0 & 0 & \frac{1}{1 - \delta^2} \end{pmatrix}$$
(4)

Then the  $C_{44}$  is fitted as the following:

$$\Delta E(V) = 2VC_{44}\delta^2 + O\left[\delta^4\right] \tag{5}$$

For cubic lattices, there are only three independent elastic constants  $C_{44}$ ,  $C_{11}$  and  $C_{22}$ .  $C_{11}$  and  $C_{22}$  can be derived as the following:

$$B = \frac{1}{3}(c_{11} + 2c_{12}) \tag{6}$$

$$c' = \frac{1}{2}(c_{11} - c_{12}) \tag{7}$$

The polycrystalline elastic moduli were derived from the single elastic constants with averaging methods. Based on the Hill averaging method [29,30], the shear modulus is derived as the following:

$$G = \frac{G_{\rm V} + G_{\rm R}}{2} \tag{8}$$

where  $G_V$  and  $G_R$  are the upper and lower bounds based on the Voigt [31] and Reuss [32] method, respectively.

$$G_{\rm V} = \frac{c_{11} - c_{12} + 3c_{44}}{5} \tag{9}$$

$$G_{\rm R} = \frac{5(c_{11} - c_{12})c_{44}}{4c_{44} + 3(c_{11} - c_{12})} \tag{10}$$

Using the derived bulk modulus *B* and shear modulus *G*, the polycrystalline Young's modulus *E* and Poisson ratio  $\nu$  can be derived as the following:

$$E = \frac{9BG}{3B+G} \tag{11}$$

$$\nu = \frac{3B - 2G}{2(3B + G)} \tag{12}$$

# 3. Results and Discussions

# 3.1. Elastic Properties of FeCr<sub>20</sub>Ni<sub>8</sub>

As listed in Table 1, the calculated bulk modulus (*B*) and shear modulus (*G*) for FeCr<sub>20</sub>Ni<sub>8</sub> are 161.8 and 77.3 GPa, respectively. These values coincide with the EMTO data published by Vitos et al. [16]. Experimental measurements of bulk modulus (*B*) and shear modulus (*G*) require dedicated techniques, so the available experimental data are very limited. As listed in Table 1, the experimentally measured bulk modulus (*B*) and shear modulus (*G*) for FeCr<sub>19.7</sub>Ni<sub>8.9</sub> are 158.2 and 77.4 GPa, respectively. Furthermore, the calculated equilibrium V<sub>0</sub> is 11.75 Å<sup>3</sup>, coinciding well with the EMTO data (11.75 Å<sup>3</sup>) [16] and experimental data (11.83 Å<sup>3</sup>) [33].

Composition at.%	V	E <sub>BCC</sub> -E <sub>FCC</sub>	<i>C</i> <sub>11</sub>	<i>C</i> <sub>12</sub>	C44	В	G	B/G	Ε	v
FeCr <sub>20</sub> Ni <sub>8</sub>	11.75	-14.01	206.8	139.3	133.1	161.8	77.3	2.09	199.9	0.29
FeCr <sub>20</sub> Ni <sub>8</sub>	11.75 <sup>a</sup>	-	208.6 <sup>a</sup>	143.5 <sup>a</sup>	132.8 <sup>a</sup>	165.2 <sup>a</sup>	77.3 <sup>a</sup>	2.13 <sup>a</sup>	-	-
FeCr <sub>19.7</sub> Ni <sub>8.9</sub>	11.83 <sup>b</sup>	-	-	-	-	158.2 <sup>c</sup>	77.4 <sup>c</sup>	2.04 c	199.6	0.29
FeCr <sub>20</sub> Ni <sub>8</sub> Mo <sub>1</sub>	11.85	-17.28	207.4	143.6	130.2	164.9	74.6	2.21	194.3	0.30
FeCr <sub>20</sub> Ni <sub>8</sub> Mo <sub>2</sub>	11.95	-20.68	208.6	146.5	126.9	167.2	72.7	2.30	190.4	0.31
FeCr <sub>20</sub> Ni <sub>8</sub> Nb <sub>1</sub>	11.88	-18.31	206.7	143.0	128.9	164.2	74.1	2.22	193.1	0.30
FeCr <sub>20</sub> Ni <sub>8</sub> Nb <sub>2</sub>	12.01	-22.99	206.5	146.9	125.7	166.7	71.1	2.34	186.8	0.31
FeCr <sub>20</sub> Ni <sub>8</sub> Ta <sub>1</sub>	11.88	-18.78	206.2	142.5	128.1	163.7	73.8	2.22	192.5	0.30
FeCr <sub>20</sub> Ni <sub>8</sub> Ta <sub>2</sub>	12.01	-23.13	204.3	146.8	125.1	165.9	70.0	2.37	184.1	0.32
FeCr <sub>20</sub> Ni <sub>8</sub> Ti <sub>1</sub>	11.81	-17.82	205.0	141.6	129.7	162.7	74.3	2.19	193.3	0.30
FeCr <sub>20</sub> Ni <sub>8</sub> Ti <sub>2</sub>	11.88	-21.77	204.4	143.1	125.2	163.5	71.7	2.28	187.6	0.31
FeCr <sub>20</sub> Ni <sub>8</sub> V <sub>1</sub>	11.77	-16.60	207.1	141.0	130.4	163.0	75.7	2.16	196.5	0.30
FeCr <sub>20</sub> Ni <sub>8</sub> V <sub>2</sub>	11.80	-19.32	205.5	143.5	128.1	164.2	73.1	2.25	190.8	0.31
FeCr <sub>20</sub> Ni <sub>8</sub> W <sub>1</sub>	11.91	-17.28	208.0	143.6	131.1	165.0	75.2	2.19	195.8	0.30
FeCr <sub>20</sub> Ni <sub>8</sub> W <sub>2</sub>	12.02	-20.54	209.2	147.7	128.9	168.2	73.1	2.30	191.6	0.31
FeCr <sub>20</sub> Ni <sub>8</sub> Zr <sub>1</sub>	11.93	-19.86	205.1	142.3	127.9	163.2	73.4	2.22	191.4	0.30
FeCr <sub>20</sub> Ni <sub>8</sub> Zr <sub>2</sub>	12.10	-25.03	203.5	144.8	123.1	164.3	69.8	2.35	183.5	0.31

**Table 1.** Calculated equilibrium unit cell volume (*V*) in Å<sup>3</sup>; the energy difference between body-centered cubic (BCC) and face-centered cubic (FCC) structure ( $E_{BCC}-E_{FCC}$ ) in mJ;  $C_{11}$ ,  $C_{12}$ ,  $C_{44}$ , bulk modulus *B*, shear modulus *G* and Young's modulus (*E*) in GPa; *B*/*G* ratio and Poisson ratio  $\nu$  are listed.

<sup>a</sup> EMTO calculated data form [16]; <sup>b</sup> Experimental data from reference [33]; <sup>c</sup> Experimental data from reference [34].

### 3.2. Solutes Effects on the Elastic Properties of FeCr<sub>20</sub>Ni<sub>8</sub>

As shown in Figure 1a, all the alloying elements considered here decrease the shear modulus (*G*) of FeCr<sub>20</sub>Ni<sub>8</sub>. For FeCr<sub>20</sub>Ni<sub>8</sub>, the shear modulus (*G*) is 77.3 GPa. The addition of 1 at.% X (X = Mo, Nb, Ta, Ti, V, W and Zr) decrease the shear modulus (*G*) by 2.7, 3.2, 3.4, 3.0, 1.6, 2.1 and 3.9 GPa, respectively. Increasing the solute concentration to 2 at.% further decreases the shear modulus (*G*) by 1.9, 2.9, 3.8, 2.6, 2.6, 2.0 and 3.5 GPa, respectively. Experimentally, adding 1.2 at.% Mo into commercial steel grades (SAE 310, 316) decreases the shear modulus (*G*) [35]. Furthermore, EMTO results also revealed that the shear modulus (*G*) of FeCr<sub>18</sub>Ni<sub>24</sub> would be decreased by the addition of Mo, Nb and V [10].



**Figure 1.** (a) Solute effects on the shear modulus (*G*). (b) Solute effects on the energy difference between the body-centered cubic (BCC) and the face-centered cubic (FCC), ( $E_{BCC}-E_{FCC}$ ).

It is believed that the shear modulus (*G*) of a face-centered cubic (FCC) metal is related to the energy difference between the body-centered cubic (BBC) and the face-centered cubic (FCC) structure,  $E_{BCC}-E_{FCC}$  [16,36].  $\Delta(E_{BCC}-E_{FCC})$  is defined as the following:

$$\Delta(E_{BCC}-E_{FCC}) = (E_{BCC}-E_{FCC})_{FeCr_{20}Ni_8X} - (E_{BCC}-E_{FCC})_{FeCr_{20}Ni_8}$$
(13)

Based on this definition, a lower value of  $\Delta(E_{BCC}-E_{FCC})$  means lower stability of the austenitic phase. As shown in Figure 1b, all the alloying elements considered here decrease the stability of the austenitic phase. This coincides with the fact that Mo, Ta, Ti, Nb, V and W are ferrite-promoting elements [37]. The addition of 1 at.% X (X = Mo, Nb, Ta, Ti, V, W and Zr) decrease the  $\Delta(E_{BCC}-E_{FCC})$  from 0 to -3.3, -4.3, -4.8, -3.8, -2.6, -3.3 and -5.9 eV, respectively. Increasing the solute

concentration to 2 at.% further decreases the  $\Delta(E_{BCC}-E_{FCC})$  to -6.7, -9.0, -9.1, -7.8, -5.3, -6.5 and -11.0 eV, respectively.

Let us shift the focus onto bulk modulus (*B*). As shown in Figure 2a, all the alloying elements considered here increase the bulk modulus (*B*) of FeCr<sub>20</sub>Ni<sub>8</sub>. For FeCr<sub>20</sub>Ni<sub>8</sub>, the bulk modulus (*B*) is 161.8 GPa. The addition of 1 at.% X (X = Mo, Nb, Ta, Ti, V, W and Zr) increase the bulk modulus (*B*) by 3.1, 2.4, 1.9, 0.9, 1.2, 3.2 and 1.4 GPa, respectively. Increasing the solute concentration to 2 at.% further increases the bulk modulus (*B*) by 5.4, 4.9, 4.1, 1.7, 2.4, 6.4 and 2.5 GPa, respectively. Experimentally, adding 1.2 at.% Mo into commercial steel grades (AISI 310, 316) increases the bulk modulus (*B*) [35]. Furthermore, EMTO results also revealed that the bulk modulus (*B*) of FeCr<sub>18</sub>Ni<sub>24</sub> would be increased by the addition of Mo, Nb and V [10].



Figure 2. (a) Solute effects on the bulk modulus (B). (b) Solute effects on the *B*/*G* ratios.

Solutes effects on the *B*/*G* ratios are shown in Figure 2b. All the alloying elements considered in this study increase bulk modulus (*B*) and decrease the shear modulus (*G*). Consequently, these alloying elements should increase the values of *B*/*G* ratio. For FeCr<sub>20</sub>Ni<sub>8</sub>, the *B*/*G* ratio is 2.09. The addition of 1 at.% X (X = Mo, Nb, Ta, Ti, V, W and Zr) increase the B/G ratio by 0.117, 0.123, 0.123, 0.096, 0.061, 0.100 and 0.130, respectively. Increasing the solute concentration to 2 at.% further increases the *B*/*G* ratio by 0.206, 0.249, 0.275, 0.186, 0.153, 0.205 and 0.259, respectively.

## 3.3. Design Map of FeCr<sub>20</sub>Ni<sub>8</sub> Based Alloys

AISI 304 stainless steel is the most common stainless steel. However, it suffered from intergranular corrosion and stress corrosion cracking when exposed to elevated temperature (500–800 °C) [5–7]. Under these environments, Cr-carbides and Cr-carbontrides precipitate at the grain boundaries, which results in the formation of a Cr-depleted zone. Potentially, alloying elements (such as Mo, Nb, Ta, Ti, V, W and Zr) might be added into austenitic stainless steels to modify the precipitate processes. Taking Ti and V as examples, the formation energies of  $Ti_{23}C_6$ ,  $V_{23}C_6$  and  $Cr_{23}C_6$  are -268, -292 and -105 meV/atom, respectively [38]. This means the addition of Ti and V will suppress the Cr-carbides and Cr-carbontrides [5,39].

On the one hand, the addition of Mo, Nb, Ta, Ti, V, W and Zr increase the bulk modulus (*B*). Higher values of bulk modulus (*B*) correspond to stronger atomic bonds, which results in better resistance to various forms of localized corrosion, such as intergranular corrosion, pitting corrosion and stress-corrosion cracking [10,12–14]. On the other hand, these alloy elements might decrease the shear modulus (*G*). Based on the simulated shear modulus (*G*) and bulk modulus (*B*), we proposed a design map of FeCr<sub>20</sub>Ni<sub>8</sub> based alloys. As shown in Figure 3, from left to right, the hardness of annealed alloys could be increased. While, from bottom to top, the resistance to various forms of localized corrosion in various austenitic stainless steels [40–42]. This design map could provide a basis for the design of high-performance austenitic stainless steels. All alloying elements considered in this work increase the corrosion resistance and ductility of the FeCr<sub>20</sub>Ni<sub>8</sub> matrix. When using this design map, we should keep in mind the reaction between the selected

alloying element and the master alloy must be taken into account. Moreover, the dosage of the alloying element should be dedicatedly controlled to avoid the formation of brittle participates [1].



**Figure 3.** Design map of FeCr<sub>20</sub>Ni<sub>8</sub> based alloys. From left to right, the hardness of annealed alloys could be increased. From bottom to top, the resistance to various forms of localized corrosion could be enhanced.

### 4. Conclusions

Using the exact muffin-tin orbitals (EMTO) method, we studied the elastic properties of  $FeCr_{20}Ni_8X_n$  (X = Mo, Nb, Ta, Ti, V, W and Zr) austenitic stainless steels. The solute concentrations considered in this work were 1 at.% and 2 at.%. All the alloying elements considered in this study increase bulk modulus (*B*) but decrease the shear modulus (*G*). As a consequence, these alloying elements should increase the values of *B*/*G* ratio. Based on the simulated shear modulus (*G*) and bulk modulus (*B*), we proposed a design map for FeCr<sub>20</sub>Ni<sub>8</sub>-based alloys, aiming to provide a basis for the design of high-performance austenitic stainless steels.

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