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Mechanical Properties and Defective Effects of 316LN Stainless Steel by First-Principles Simulations

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In current International Thermonuclear Experimental Reactor (ITER) design, the 316LN austenitic stainless steel (316LN SS) is used for first-wall/blanket structures. Thus, it is necessary to study the fundamental mechanical properties and irradiation effect of 316LN SS. A random solid solution model of Fe-Cr-Ni-Mn-Mo-Si alloy is used for describing 316LN SS. Using first-principles approaches, the elastic constants and ideal strength of the alloy were calculated. Such alloy exhibits good ductile behavior according to the theoretical values of Cauchy pressure and ratio of bulk modulus and shear modulus. Within the 256-atom supercell, inclusion of single vacancy defect further enhances the ductility of the alloy, and the existence of interstitial (Fe, H, He) atoms enhances the Young′s modulus.

KEY WORDS: Stainless steel; Mechanical properties; Vacancy; Interstitial

1. Introduction

Austenitic stainless steels composed of Fe, Cr, and Ni as well as other trace elements like Mo, Si, Al exhibit excellent corrosion resistance, fine strength, toughness and plasticity. Among them the 316LN austenitic stainless steels with main elements of Fe, Cr, Ni, Mn, Mo, Si are considered to have good thermal and mechanical properties, and currently serve as the primary structural materials in the first wal1 and blanket structure of the International Thermonuclear Experimental Reactor (ITER)[1–6]. Under ITER working conditions, structural materials are directly exposed to 14 MeV neutron irradiation at high temperature of about 600 K. Therefore, it is crucial to study the fundamental mechanical properties and irradiation effect of the 316LN SS from the safety point of view.

It is well known that the elastic modulus of a material are able to characterize the mechanical deformation and structural stability under external loading[7,8]. In addition to the elastic behavior, the ratio of bulk modulus and shear modulus (B/G) and the Cauchy pressure ($C_{12}-C_{44}$)/2 are usually employed to assess the ductile/brittle characteristics of a material[9,10]. Previously, the elastic properties of the austenitic stainless steels have been studied from both experimental and theoretical sides. Most of experimental works focused on the effects of temperature, pressure, and chemical composition on elastic constants[11–17]. For example, Sudook *et al.*[17] measured the elastic constants of four types of Fe-Cr-Ni-Mn alloys, which contained 16–23 at.% Cr, 7–28 at.% Ni, and 0–13 at.% Mn, and found that both Cr and Ni increase the bulk modulus and decrease the shear modulus. Previous theoretical works also focused on the variation of elastic properties with chemical compositions[18–20]. For instance, Vitos *et al.*[19] mapped the elastic properties of austenitic stainless steels as a function of Ni and Cr compositions and predicted two basic compositions with outstanding mechanical properties among the austenitic stainless steels.

Under the ITER working condition, 14 MeV neu-

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Table 1 Chemical composition of 316LN austenitic stainless steel (316LN SS) in experiment and our random solid solution model with 256 atoms ($Fe_{165}Ni_{34}Cr_{48}Mn_3Si_3Mo_3$), in wt%

316LN SS	C	S	P	Si	Mn	Cr	Ni	Mo	Fe
Expt.[30]	0.03	0.03	0.045	1.0	2.0	16.0–18.0	10.0–14.0	2.0–3.0	Bal.
This work	–	–	–	0.59	1.16	17.52	14.01	2.02	Bal.

tron irradiation would inevitably induce structural defects such as vacancies, interstitials, voids and bubbles[21–25]. All these defects are expected to affect the mechanical properties of the stainless steels. At present, there have been some experimental efforts in understanding the irradiation effects on the mechanical properties of the austenitic stainless steel[26–29]. For instance, Hunn *et al.*[29] irradiated the 316LN SS with He ions and found that the He bubbles caused hardening of the steel. Hashimoto *et al.*[28] measured the mechanical strengths of 316LN SS irradiated with the neutrons and discovered that the yield strength increases with the production of vacancy and interstitial clusters.

To our knowledge, there has been no theoretical study on the effect of the individual vacancy or interstitial defect on the mechanical properties of the 316LN SS, which is very useful to establish a microscopic picture of the neutron irradiation effect. Furthermore, the ductile/brittle behavior as well as the ideal strength of the 316LN SS have not been examined from the theoretical point of view. In this work, considering the structural complexity of 316LN SS, a solid solution model of the 316LN SS including its main constituent elements of Fe-Cr-Ni-Mn-Mo-Si is introduced to evaluate the effect of point defects and mechanical properties.

2. Model and Computational Methods

The standard chemical composition of the 316LN SS[30] is given in Table 1. As shown in Table 1, the minor elements of C, S and P are not considered in the present models of 316LN SS since their respective atomic number in a 256-atom face cubic-center supercell is less than one. The random solution solid model can be constructed by different methods[31–33]. For example, Zunger *et al.*[31] used the model of "special quasirandom structure" (SQS's), a random network considering the close neighbors around a given site, to characterize a number of semiconductor alloys. In this work, due to the complexity of the multicomponent system (as shown in Table 1), the effect of heat of mixing[32] was taken into account to construct the random solid solution model of 316LN SS, that is, if the heat of mixing for two elements is negative, these two elements prefer to aggregate; otherwise, they tend to separate in the solid solution. Within a cubic supercell of the face-center cubic (fcc) lattice, the random solid solution model with 256 atoms (4×4×4 unit cells) were constructed for the 316LN SS, in which a certain amount of Fe atoms was substituted randomly by Ni, Mn, Cr, Si and Mo atoms to meet the stoichiometry of $Fe_{165}Ni_{34}Cr_{48}Mn_3Si_3Mo_3$. For this stoichiometry, a number of random configurations were generated and the one with the lowest energy after first-principles optimization was selected for further simulation of the mechanical properties.

First-principles calculations were performed using density functional theory (DFT)[34] and projector-augmented wave (PAW) method[35,36] as implemented in the Vienna Ab-initio Simulation Package (VASP)[37]. We adopted the generalized gradient approximation (GGA) of the Perdew and Wang (PW91) functional to describe the exchange-correlation interaction[38]. A cutoff energy of 400 eV was used for plane wave basis. Further increasing cutoff energy has only a little effect on computational results. Due to the large lattice dimension, we used Γ point to sample the reciprocal space for the 256-atom supercell of Fe and Fe-based alloy. For comparison, we computed the fcc Fe with one unit cell and 10×10×10 k point meth. The theoretical lattice constant and bulk modulus for fcc Fe are 0.3446 nm and 302 GPa respectively from unit cell calculations, which agree reasonably well with 0.3442 nm and 286 GPa from supercell calculations.

For a cubic crystal, there are only three independent elastic constants (C_{11}, C_{12}, C_{44}), which can be obtained by applying suitable deformation gradient tensors F on the simulation supercell:

$$F = I + \varepsilon \tag{1}$$

where I is the identity matrix, ε is the 3×3 strain tensor and

$$\varepsilon = \begin{pmatrix} e_1 & e_6 & e_5 \\ e_6 & e_2 & e_4 \\ e_5 & e_4 & e_3 \end{pmatrix} \tag{2}$$

To determine the three independent elastic constants C_{11}, C_{12}, and C_{44}, here we chose three sets of strain tensors as below:

$$\begin{bmatrix} \delta & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{3}$$

$$\begin{bmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \delta \end{bmatrix} \tag{4}$$

$$\begin{bmatrix} 0 & \delta & \delta \\ \delta & 0 & \delta \\ \delta & \delta & 0 \end{bmatrix} \tag{5}$$

Table 2 Calculated bulk modulus (B), shear modulus (G), Young′s modulus (E), Possition ratio ν, Cauchy pressure $(C_{12}-C_{44})/2$, and B/G ratio of fcc Fe solid. Previous experimental and theoretical values are also shown for comparison

	a_0/nm	B/GPa	G/GPa	E/GPa	ν	$(C_{12}-C_{44})/2$ /GPa	B/G
256 atoms	0.3442	286	144	370.0	0.28	23.0	2.0
FLAPW[41]	0.3450	317	240	575.0	0.20	– – 26.5	1.3
FLAPW[42]	–	260	240	550.0	0.15	– – 70.0	1.1
EMTO[43]	–	300	172.7	434.7	0.26	–19.5	1.74
PAW-LDA[44]	0.3382	320	–	–	–	–	–
Expt.[45,46]	0.3660	133	53	140.0	0.32	22.5	2.5

where δ is the strain parameter. Based on the continuum elasticity theory[39,40], the strain energy density can be expressed as an expansion by the parameter δ:

$$\rho_0 \left[U\left(\delta\right) - U\left(0\right)\right] = \frac{1}{2}A_2\delta^2 + \frac{1}{6}A_3\delta^3 + O\left(\delta^4\right) \quad (6)$$

where U_0 $(U(\delta))$ is the internal energy of the initial (strained) states, ρ_0 is the initial mass density of the material, the coefficients are the combinations of second- and third-order elastic constants of the crystal, respectively. In the case of small deformation ($\delta \leq 1\%$), we can fit Eq. (6) up to quadratic term, thus the elastic energy density associated with strain tensors described by Eqs. (3)–(5) are given by:

$$\rho_0[U(\delta) - U(0)] = \frac{1}{2}C_{11}\delta^2 \quad (7)$$

$$\rho_0[U(\delta) - U(0)] = \frac{3}{2}(C_{11} + 2C_{12})\delta^2 \quad (8)$$

$$\rho_0[U(\delta) - U(0)] = 6C_{44}\delta^2 \quad (9)$$

respectively. Based on the elastic constants C_{11}, C_{12}, and C_{44} calculated from Eqs. (7)–(9), the bulk modulus (B), isotropic shear modulus (G), isotropic Young′s modulus (E), Cauchy pressure (C'), and Poisson′s ratio ν can be obtained from the following relations:

$$B = (C_{11} + 2C_{12})/3 \quad (10)$$

$$G = (3C_{44} + C_{11} - C_{12})/5 \quad (11)$$

$$E = 9BG/(3B + G) \quad (12)$$

$$C' = (C_{12} - C_{44})/2 \quad (13)$$

$$\nu = (E/2G) - 1 \quad (14)$$

3. Results and Discussion

To assess the reliability of our computational methods, we first investigated the fundemental properties of fcc solid of pure paramagnetic iron. For pure paramagnetic iron, there have already been numerous theoretic methods with different functions for the calculation of elastic moduli of fcc Fe crystal, such as FLPAW method with generalized gradient approximation (GGA), PAW method with local density approximation (LDA), and Exact Muffin-Tin Orbital Method (EMTO) with coherent potential approximation. All of the previous theoretical results calculated by these methods[41–44], together with experimental ones, are shown in Table 2[45,46]. With regards to the experimental data, our theoretical calculations overestimate the elastic moduli to certain extent. But our current results are closer to experimental values comparing with previous calculations using FLPAW method with the generalized gradient approximation (GGA). Meanwhile, the values of the lattice constants a_0(0.3442 nm), the ratio B/G (2.0), Cauchy pressure $(C_{12}–C_{44})/2$ (23 GPa), and Poisson′s ratio ν (0.28) from our calculations deviated from the experimental values by about 6%, 20%, 2%, 12.5%, respectively. Overall speaking, our present method is able to describe the mechanical properties of 316LN SS and the irradiation effects at least in a qualitative manner.

As the structural material for the first-wall and blanket in fusion reactor, the 316LN SS will be directly exposed to the 14 MeV neutron irradiation. Therefore, vacancies, interstitial atoms (like Fe) or impurities (H, He) will be introduced under neutron irradiation, which will further influence their mechanical properties. To understand such defective effects on the mechanical properties of 316LN SS, here we simulated the mechanical properties of the defective crystals containing only one vacancy or one interstitial (Fe, H, He) defect per supercell. The theoretical results are given in Table 3. Compared with the Young′s modulus (E) of the perfect crystal of 316LN SS, the existence of single interstitial (Fe, H, He) defects would enhance the Young′s modulus by about 16–19 GPa, but the crystal with single vacancy defects show no obvious variation in the E value.

It is known that the ductility/brittleness plays a key role in determining the mechanical performance of a material, which can be roughly evaluated by the ratio of bulk and shear modulus (B/G)[9] and the Cauchy pressure $(C_{12}–C_{44})/2$[10]. According to Pugh′s proposal[9], if the B/G ratio of a material is greater than 1.75, the material behaves in a ductile manner, otherwise a brittle manner. The Cauchy pressure has a positive value if the bonding in the ductile materials shows more metallic character (*e.g.*, Al, Ni), whereas with angular or directional bonding characteristics the Cauchy pressure of a cubic crystal (such as the brittle semiconductor Si, Ge) will be neg-

Table 3 Calculated Young′s modulus (E), Possition ratio ν, Cauchy pressure $(C_{12}-C_{44})/2$, and B/G ratio of fcc 316LN stainless steel. Previous experimental values are also shown for comparison

	a_0/nm	E/GPa	ν	B/G	$(C_{12}-C_{44})/2$ /GPa
Perfect	0.3490	338.0	0.29	2.02	23.0
Expt.[5,48]	0.3598	199.6	0.29	2.06	–
Cr vacancy	–	345.8	0.32	2.09	28.0
Fe vacancy	–	336.8	0.30	2.11	29.0
Ni vacancy	–	346.4	0.31	2.08	31.5
Mn vacancy	–	329.0	0.30	2.09	28.0
Fe interstitial	–	354.6	0.29	2.06	27.3
H interstitial	–	355.3	0.29	2.02	24.4
He interstitial	–	357.0	0.29	2.02	23.9

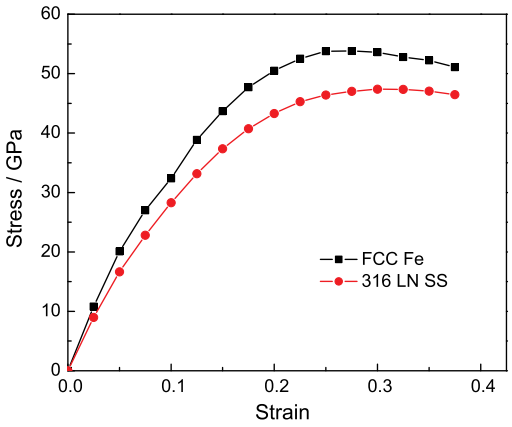

Fig. 1 Stress–strain relationships for 316LN stainless steel and pure fcc Fe solid under tensile strains

ative. As shown in Table 3, the B/G ratio (2.02) of the 316LN SS is higher than the critical value of 1.75, indicating that the 316LN SS have excellent ductile characteristic. This is also supported by the positive value of Cauchy pressure (23 GPa).

We further discussed the defective effects on the ductile/brittle behaviors. Although the single vacancy defect has less effect on the Young's modulus (E), it can improve the ductility of the 316LN SS solid, which can be seen from the calculated values of B/G and Cauchy pressure (see Table 3) of the defective crystal structures. Interestingly, all interstitial (Fe, H, Fe) atoms show little effect on the ductile behavior of 316LN SS. Experimentally, the ductile characteristic of the 316LN SS was usually reduced after neutron irradiation[23]. However, revealed by MD simulations[47] of the silicon carbide systems, the ductility can vary with different irradiation doses. The various defect types accumulated at diverse dose levels suggest that such irradiation-induced downgrade of ductility is not simply originated from the individual structural defects like vacancies, interstitial atoms. Instead, the location loops, voids and bubbles[22,25] due to accumulation of these structural defects might be more important for determining the macroscopic ductile behavior of the 316LN SS.

We also examine the ideal strength of the 316LN SS, which is defined as the minimum stress needed to force deformation or fracture of a perfect crystal. In this work, the ideal tensile strength of 316LN SS and pure paramagnetic fcc Fe solid along [100] direction were investigated by applying a series of tensile strains and computing the corresponding stress components along this direction. The calculated stress–strain relationships for 316LN SS and pure Fe of fcc phase are shown in Fig. 1. One can see clearly that the stress first increases with increasing strain, and then decreases after reaching a maximum of 53.8 GPa at a critical strain of 27.5% for fcc Fe and a maximum stress of 47.4 GPa at 30% for 316LN SS. From the difference in the critical strains, the pure fcc Fe is more brittle than 316LN SS.

4. Conclusion

First-principles calculations within the random solid solution models have been performed to investigate the fundamental mechanical properties of 316LN SS and discussed the effects of vacancy and interstitial defects. According to our theoretical results, the 316LN SS exhibit good ductility, as justified by the high B/G value, positive Cauchy pressure, and appreciable ideal strength. The existence of individual interstitial atoms would enhance the Young′s modulus of the 316LN SS but result in no significant modification to the ductile property. On the contrary, inclusion of the single vacancy defect shows obvious effect on the ductility and little contribution to Young′s modulus. These results may provide some useful insights in the fundamental mechanical properties and irradiation damage of the 316LN SS.

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