Comparative study on the strain-dependent mechanical and electronic properties of Nb$_3$Al and Nb$_3$Sn

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Abstract

Nb$_3$Al and Nb$_3$Sn are important A15 compounds due to their good superconducting properties in high magnetic field. The strain coming from multiple sources would result in the degradation of superconducting performance for both of them. Extensive experimental studies have found that Nb$_3$Sn has higher strain sensitivity than Nb$_3$Al. However, most of the previous theoretical works focus on the effect of compressive hydrostatic pressure, which doesn’t reflect the actual working condition. In this work, first-principles calculations were done to investigate the mechanical behaviors of the two materials under the three crystallographic uniaxial tensile loadings. Determined from the stress-strain relations, the theoretical strength of Nb$_3$Al is found to be slightly higher than that of Nb$_3$Sn, which is validated by the energy-strain curve and the corresponding phonon instability. Electronic analyses show that the property difference of the two materials is attributed to their different bonding states and strain sensitivities. The present work unveils why the superconductivity of Nb$_3$Sn is more sensitive to strain than Nb$_3$Al on the microscopic level.

1. Introduction

Nb$_3$Al and Nb$_3$Sn are important intermetallic compounds owing to their good superconducting properties in the liquid helium temperature range [1–3]. Their high critical current densities in high fields enable them to be applied as superconducting magnets on large-scale applications, such as nuclear fusion, high-energy accelerators and gigahertz class nuclear-magnetic-resonance (NMR) [4, 5]. For example, thanks to the commercially available fabrication process, Nb$_3$Sn has already been applied as the superconducting material for magnets on the International Thermonuclear Experimental Reactor (ITER) [6–8]. However, the better strain tolerance of Nb$_3$Al makes it an ideal alternative to Nb$_3$Sn for high-field applications [9, 10], although the commercialization of its fabrication is still challenging [11]. Considerable efforts have been devoted to fabricating Nb$_3$Al with right stoichiometry and stable superconducting properties under high magnetic fields [12–16].

For application of Nb$_3$Al or Nb$_3$Sn as superconducting magnets, they are usually made of multifilamentary strands which form a cable with complex architecture to fulfill the desired engineering characteristics [17–21]. Take the Cable-In-Conduit (CIC) conductors for the Toroidal Field (TF) and Center Solenoid (CS) coils in the ITER as example, there are more than 1000 Nb$_3$Sn strands in them [22, 23]. Each of the single strand has a diameter of less than 2 mm. As for the architecture, a typical cable is made of the functioning superconducting multifilamentary strands plus additional components, such as the metal matrix material and stabilizers [5]. Because of the different thermal expansion coefficients and elastic moduli of these components, there are complicated local strain/stress distributions in the superconducting material which may have considerable influence on the mechanical and superconducting properties [24, 25]. In addition to this, during the operation of the superconducting magnets, the cable will experience transverse Lorentz force, which is substantially large when the working magnetic field is huge (> 11 Tesla) [26, 27]. The strain results from the manufacture and
operation can lead to the performance degradation or even filament breakage. Therefore, it is necessary to study their mechanical properties of the two important candidate materials under strain.

Many previous theoretical works have studied the properties change of Nb3Al and Nb3Sn under hydrostatic pressure which is compressive strain [28–30]. However, for the application of superconductor magnets, the superconducting materials not only undergo compressive strain but also tensile strain. For example, when the Nb3Al or Nb3Sn superconducting strands are fabricated, the widely adopted methods like Rod-in-tube, Clad-chip extrusion or Powder-in-tube would result in large tensile strain in the materials [1, 31, 32]. Furthermore, when theses superconducting strands are utilized in the magnets, strand bending results from the manufacture process or Lorentz force during operation would also lead to the tension state in the materials. In light of this, it is of great importance to study the mechanical and electronic properties of Nb3Al and Nb3Sn under tensile strain.

In this work, we use first-principles simulations based on density functional theory (DFT) to investigate the mechanical properties of Nb3Al and Nb3Sn. Unlike many of previous studies, where hydrostatic pressure were applied, we simulated the mechanical behaviors of the two materials under the three low-index crystallographic uniaxial tensile loadings. Combining the stress-strain relations, energy-strain relations and the phonon dispersion analysis, it is determined that Nb3Al possesses slightly higher theoretical strength than Nb3Sn. The structural evolution and failure mechanism of the two materials under uniaxial tensile loadings were also studied. Most importantly, the strain-dependent electronic sensitivities of them are studied by detailed electronic analyses. The results in this work provide deeper understanding on the atomic level that why Nb3Al has better strain tolerance than Nb3Sn in terms of their superconducting performance.

2. Computational methods

All the first-principles calculations in this work were done based on DFT using the VASP package [33]. PBE functional under the frame of generalized gradient approximation (GGA) was used. Projector augmented wave (PAW) method was used to describe the electronic structures of the three elements, Nb, Sn and Al. An energy cutoff of 450 eV was used to truncate the plane-wave expansion for both Nb3Al and Nb3Sn. The Γ-centered k-point grids with a density equivalent to that of 8 × 8 × 8 was used for the integrations of the Brillouin zone. The conjugate-gradient algorithm was used for the geometry relaxation of the structures under different strains. The electronic self-consistent field (SCF) convergence threshold was 1 × 10−6 eV while the tolerance for the forces acting on the atoms was less than 0.01 eV Å−1. The strain-stress curve was obtained by plotting the stress of the unit cell corresponding to its strain. The uniaxial tensile strain was manually applied to the unit cell of the two materials step by step. While the stress was defined as the Hellmann-Feynman stress. Many previous works have used such method to effectively study the mechanical properties and theoretical strength of materials [34–36]. The electron localization function was calculated using VASP and the corresponding 2D plot was done in VESTA [37]. The phonon dispersions of the structures were calculated by PHONOPY [38] code interfaced with VASP, where the force constant matrices were obtained by density functional perturbation theory (DFPT) from a non-displaced 2 × 2 × 2 supercell constructed by PHONOPY.

3. Results and discussion

Figure 1 shows the crystal structures of Nb3Al and Nb3Sn, both of which possess the typical A15 crystal structure where the Al or Sn forms a body-centered cubic (BCC) structure while there are two Nb atoms on each of the six
surfaces. Alloys that have A15 structure are usually superconductors and are mechanically brittle [39]. In the present work, the lattice constants of them are calculated to be 5.19 Å and 5.31 Å, respectively, which are in good agreement with previous theoretical results [40, 41], validating the reliability of the calculations in this work. In order to study the structural evolution under uniaxial tensile loadings in the following discussion, the two bonds, d1 and d3, between Al(Sn)-Al(Sn) and one bond d2 between Al(Sn)-Nb are labeled as well as the angles of $\theta_1$ and $\theta_2$ between Nb-Al(Sn)-Nb and Al(Sn)-Al(Sn)-Al(Sn), as shown in figure 1.

The theoretical strength of a material is closely related to its crystal structure and is a fundamental mechanical property which reflects its nature of chemical bonding. By means of first-principles simulations, the theoretical strength of a material can be determined from the stress-strain curve where the maxima on the curve indicates the theoretical strength [42]. Figure 2 shows the stress-strain relations of Nb$_3$Al and Nb$_3$Sn under uniaxial tensile loadings along the three low-index crystallographic directions. The data show that the mechanical behaviors of the two materials show strong similarities because of their similar crystal structure. Both of them possess the highest theoretical strength along [100] direction, while the lowest theoretical strength is along [110]. Before reaching the theoretical strength, the stress monotonically increases with the loading strain, suggesting that the structures uniformly resist the tension by deformation along the loading direction. In addition, during the elastic deformation process before strain of 0.2, there is little anisotropy among the three directions in both of them, which suggest that both Nb$_3$Al and Nb$_3$Sn have similar resistance to uniaxial tensile loading along the three directions, which is different from other materials with cubic crystal structure. This may be attributed to the unique A15 structure. Table 1 summarizes the theoretical strengths as well as the corresponding strains obtained from figure 2. It is noted that Nb$_3$Al has higher theoretical strength than Nb$_3$Sn under uniaxial tensile loading along all the studied directions. This is consistent with the experimental fact that Nb$_3$Al is more widely used as high-temperature structural material [43].

Although the theoretical strength of a material can be directly determined from its stress-strain relation under a specific loading mode, like in the case of figure 2, further analysis is needed to confirm the theoretical strength value. From the traditional view of mechanical stability, the theoretical strength of a material corresponds to the inflexion point on the energy versus strain curve derived from the loading process [44]. Recently, based on the stability analysis of a system from the view of thermodynamics, Wang established a strength criterion which also suggests that the theoretical strength of a material can be determined from the energy versus strain curve [45, 46]. Therefore, the energy evolution as a function of the strain during the uniaxial

![Figure 2](image-url) The calculated stress-strain relations of (a) Nb$_3$Al and (b) Nb$_3$Sn under directional uniaxial tensile strain.

| Materials | 100     | 110     | 111     |
|-----------|---------|---------|---------|
| Nb$_3$Al  | 26.41 GPa | 20.42 GPa | 23.797 GPa |
| $\varepsilon$ | 0.308 | 0.257 | 0.270 |
| Nb$_3$Sn  | 24.24 GPa | 19.67 GPa | 20.97 GPa |
| $\varepsilon$ | 0.269 | 0.257 | 0.257 |
The tensile loading process is plotted in Figure 3, where Figures 3(a)–(c) represent the loading process of Nb3Al, while Figures 3(d)–(f) represent the loading process of Nb3Sn. It is obvious that the inflexion points on each of the energy-strain curves correspond to the maximum stress values, which are the same as determined from Figure 2. The consistence of the stress-strain curve and the energy-strain curve confirms the validity of the theoretical strength calculated in this work, i.e., Nb3Al has higher theoretical strength than Nb3Sn under uniaxial tensile loading along the three low-index crystallographic directions.

To further confirm our conclusion, phonon dispersions of the structures under the strains correspond to the inflexion points were calculated and are shown in Figure 4. As was developed by previous researchers [47], the stability conditions for a perfect structure loaded under uniaxial tension hold the following relations:

\[(C_{33} + \sigma)(C_{12} + C_{13}) - 2\left(C_{13} - \frac{\sigma}{2}\right)^2 > 0\]  \hspace{1cm} (1)

\[C_{41} - C_{12} > 0\]  \hspace{1cm} (2)

\[2C_{44} + \sigma > 0\]  \hspace{1cm} (3)

\[C_{66} > 0\]  \hspace{1cm} (4)

where \(C_{ij}\) are the conventional elastic constants (in Voigt notation) and \(\sigma\) is the loaded stress. Equations (2)–(4) indicate the conditions to prevent the crystal from shear instabilities. So our focus is on the first condition which indicates the stability condition under uniaxial loadings. Violation of equation (1) is closely related to the inflexion point on the energy versus strain curve during the uniaxial loading process. Thus, it is implied that when the crystal is under the strain corresponding to the inflexion point, the structure becomes thermodynamically unstable, which is consistent with the criterion established by Wang [45]. When the system becomes unstable, it is reflected from its phonon dispersion that imaginary frequency appears [48, 49]. It can be seen from Figure 4 that there are imaginary frequencies in all the structures under the strains corresponding to the inflexion points. It has been a long debating issue that A15 structures including Nb3Al and Nb3Sn exhibit structural instabilities even at zero strain state. So people have found imaginary phonons for non-strained Nb3Al and Nb3Sn [3, 50–52]. Our calculations also show that there are negative frequencies at zero strain for both of the structures, which is consistent with previous findings. Therefore, the imaginary phonons calculated at the inflexion points can only suggest the structures are not stable. However, how the stability transformation occurs during the loading process as reflected by phonons requires a point-by-point analysis of the phonon dispersion under every strain case, which is beyond the scope of current work.

To examine the deformation and failure mechanisms of Nb3Al and Nb3Sn under uniaxial tensile loading, the typical bond lengths and angles in the structure as shown in Figure 1 were studied during the loading process.
Figures 5(a)–(c) and 5(d)–(f) display the typical bond and angle evolutions under [100] uniaxial tensile loading for Nb₃Al and Nb₃Sn, respectively. It is clearly seen that both Nb₃Al and Nb₃Sn show very similar mechanical and failure behavior during the loading process, which is consistent with their similar stress-strain relations as shown in figure 2 owing to their same crystal structure. According to the plots in figure 5, the bond lengths all increase with the uniaxial strain. As shown in figure 5(a), the bond length of d₁ increases from 5.19 Å to 6.86 Å, with a percentage of ∼32%, while the bond length of d₂ increases from 2.90 Å to 3.61 Å, with a percentage of
∼24%. In contrast, the bond length of d3 increases from 4.49 Å to 4.88 Å, with a percentage of only ∼8%. Due to the same crystal structure, the bonds evolution shares the similar feature in Nb₃Sn as shown in figure 5(d), where the bond length of d1 and d2 increase more than 20% while the bond length of d3 increases less than 10%. The large increase in the length of d1 and d2 is because they are more parallel with the uniaxial tension direction, while the small increase in the length of d3 is because it’s more perpendicular to the loading direction. These suggest that the structure is elongated when it is under uniaxial tension along the loading direction, while the size of the other two directions contract, which demonstrate that Nb₃Al and Nb₃Sn have positive Poisson’s ratios, as has been found in previous research [40, 53]. In addition, the elongation along the tension direction and contraction along the other two directions are also demonstrated by the increase in θ₂ and decrease in θ₁.

Figures 5(b) and (e) are magnified from figures 5(a) and (d), respectively, to show the non-linear trend of the d₃ bond change in Nb₃Al andNb₃Sn. It can be seen that there is acceleration in the increase of the d₃ bond length from the strain-free state to the failure strain, suggesting that the structure is gradually becoming unstable, which is consistent with the appearance of imaginary frequencies as observed in figure 4.

The above discussion show that Nb₃Al has better mechanical stability than Nb₃Sn under uniaxial tensile loadings. To further analyze the strain dependent properties of Nb₃Al and Nb₃Sn, detailed electronic analyses were conducted. Figures 6(a) and 6(b) show the DOS (density of states) and PDOS (partial density of states) of Nb₃Al and Nb₃Sn under strain-free state, respectively. The general features of them are quite similar because they share the same A15 crystal structure. In both of them, there is large DOS near the Fermi energy, indicating the metallic nature of the two materials. Furthermore, the PDOS of them suggest that the main contribution is from Nb while there is hybridization between either Nb and Al or Nb and Sn since there is noticeable PDOS from Al and Sn. Except for these similar features, the biggest difference between the DOS of the two materials is that Nb₃Sn has more localized DOS than Nb₃Al as shown in the studied energy range. Figures 6(c) and (d) show the DOS and PDOS of Nb₃Al and Nb₃Sn under the failure strain point, respectively. In contrast to the strain-free state, the general feature of the DOS for the two materials doesn’t change much. However, the center of DOS in both of them shifts towards lower energy, where there is only slight shift in Nb₃Al while there is huge shift in Nb₃Sn which results in a more localized DOS compared with its strain-free state. According to the well-established theory that the Fermi energy (E_f) of the electron gas is closely related to the volume of the structure, i.e., $E_f \propto V^{-2/3}$, where V is the volume of the structure [54]. In the case of this study, when Nb₃Al and Nb₃Sn are under uniaxial strain, the volume of the cell increases which leads to the DOS shifts to lower energy. The different DOS response to uniaxial strain demonstrates that Nb₃Sn has more sensitive strain-dependent...

![Figure 6](image-url)
electronic properties than that of Nb3Al, which may probably account for its more sensitive strain-induced superconductivity degradation.

To further study the electronic response towards uniaxial tension, the ELF (electron localization function) evolution of Nb3Al and Nb3Sn during the loading process is shown in figure 7. ELF is a measure of the possibility of finding an electron in the neighborhood space and is usually used to analyze the interatomic interaction in materials in a chemically intuitive way [55]. Conventionally, the value of ELF varies from 0 to 1, where ELF = 1 corresponds to perfect localization while ELF = 0 corresponds to completely delocalization. It can be seen in figure 7 that Nb3Sn has stronger electron localization than Nb3Al under strain free state, which is in well accordance with the DOS analyses from figure 6. What’s more important, when they are under uniaxial tension, the degree of localization in both of them increases since the dark blue areas become more obvious as shown in figures 7(c) and (f), which is also reflected in their DOS in figure 6 that the energy range of the DOS becomes narrower. In addition, when the electron localization increases, the bonding strength between the atoms weakens, which is demonstrated that the bond lengths in figure 5 increases along with the uniaxial strain. In terms of the strain-dependent sensitivity, although there is increase in the electronic localization in Nb3Al when strain changes from 0 to 0.308, the electronic localization in Nb3Sn is more obvious because the dark blue area in figure 7(f) indicates that almost complete delocalization occurs, which suggests that electrons localize stronger in the surroundings of Nb atom. Based on the above discussion, it is concluded that Nb3Sn has bad strain tolerant superconductivity than Nb3Al because the bonding between Nb and Sn is more sensitive to strain which may weaken its interaction and thus tune the electronic structure near the Fermi energy.

To confirm the validity of the conclusion drawn from the present work, we compare our results with some of the previous research. Tutuncu et al made the first attempt to study the origin of superconductivity in Nb3Sn by ab initio calculations [56]. The authors demonstrated that the superconductivity of A15 Nb3Sn comes not only from the longitudinal acoustic phonon mode but also the phonons near 4.5 THz. Although the phonon dispersions calculated in this work contain some imaginary frequencies, the vibrational modes near 4 THz is also quite dense, which is consistent with Tutuncu et al’s work. The lowered frequency is resulted from the softening of the structure due to the applied tensile strain. From the electronic point of view, our present work suggests that when strain is applied, the higher electron localization in Nb3Sn than Nb3Al accounts for its bad strain-dependent superconductivity degradation. Godeke et al have found the experimental evidence that doping of Zn into Nb3Sn can significantly increase its strain tolerance [57]. This confirms our findings because doping of Zn may introduce extra density of states near the Fermi energy and thus may improve the strain tolerance of Nb3Sn towards superconductivity degradation. Therefore, the present work studied the superconductivity strain sensitivity of Nb3Sn on the microscopic level and suggests that doping or alloying may be a solution to this issue.
4. Conclusions

In this work, the theoretical strength and electronic properties of Nb₃Al and Nb₃Sn were studied by means of first-principles methods based on density functional theory. The stress-strain relations of them were obtained by simulating the loading process under the three low-index crystallographic uniaxial tensile strain. The theoretical strength is determined as the maximum stress value on the stress-strain curve. Nb₃Al is found to have a higher theoretical strength than that of Nb₃Sn which is validated by the in flexion point on the corresponding energy-strain curve. The failure mechanism analyses suggest that the structures resist the uniaxial tension by bond length elongation which leads to the softening of the interatomic interactions, accompanied by the appearance of imaginary frequencies in the phonon dispersions. The electronic responses to uniaxial tensions were also studied which reveals that Nb₃Sn is more sensitive towards strain than Nb₃Al. It is found that electron localization in Nb₃Sn significantly increases under uniaxial tension which results in the weakened atomic interactions between Nb and Sn, thus tuning electronic properties near the Fermi energy. The present work provides reasonable explanation for the strain-dependent properties of the two materials. It may also provide a possible guidance that if the strain dependent electronic sensitivity of Nb₃Sn can be suppressed by method, such as doping or alloying, then the strain-induced superconductivity degradation may thus be prevented or alleviated.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

Declaration of competing interest

The authors declare no competing financial interests.

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