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Orientation, Size, and Temperature Dependent Ductile Brittle Transition in NiAl Nanowire under Tensile Loading - A Molecular Dynamics Study

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ABSTRACT

In the present paper, thermo-mechanical response of B2-NiAl nanowire along the <100>, <110>, and <111> orientations has been studied using molecular dynamics simulations. Nanowire with cross-sectional dimensions of ~20x20 Å^2, ~25x25 Å^2, and ~30x30 Å^2 and temperature range of 10 K-900 K has been considered. A Combined effect of size, orientation, and temperature on the stress-strain behavior under uniaxial tensile loading has been presented. It has been observed that <111> oriented *NiAl* nanowire that is energetically most stable gives highest yield stress which further reduces with <110> and <100> orientations. A remarkable ductile brittle transition (DBT) with an increase in temperature has also been reported for all the orientations considered in the present study. The DBT observed for the nanowire has also been compared with the reported DBT of bulk B2-NiAl obtained from experiments. Alternate technique has also been proposed to increase the toughness of a given material especially at lower temperature regions, i.e. below DBT.

Keywords: Intermetallic compounds, nanostructurs, molecular dynamics, mechanical properties, phase transitions, ductile brittle transition temperature.

1. INTRODUCTION

The ductile-brittle-transition (DBT) is conventionally defined as a sharp increase in the toughness of material that is evaluated at the point of crack instability[1]. The ductile-brittle transition temperature (DBTT) which is also known as nil ductility temperature (NDT) or nil ductility transition temperature (NDTT) of a material that represents a point at which the fracture energy passes below a pre-determined point. DBTT is very critical parameter in a material that operates below the DBTT because it has a greater tendency to fail via brittle fracture instead of bending or deforming plastically. DBTT is of great concern in materials selection when it is subjected to thermo-mechanical loading. NiAl is one of the materials that have been used extensively in aerospace engine applications, where thermo-mechanical loading is of great importance. The reason behind using NiAl as compared to the nickel based superalloys in aerospace engine applications are mainly

(a) density of 5.95 g/cm^3, which is approximately 1/3rd the density of state-of-the-art nickel based superalloys
(b) thermal conductivity is 4 – 8 times of nickel-based superalloys (depending upon composition and temperature)
(c) excellent oxidation resistance, and
(d) simple, B2 crystal structure makes plastic deformation potentially easier compared to many other intermetallic compounds[2].

It is well known that the low fracture toughness has a detrimental effect on the tensile ductility. Like most of the other intermetallics, unalloyed NiAl suffers from lack of ductility at low temperature and poor strength at high temperature[2]. Noebe[3], *et al.* have reported that both the poor ductility and fracture toughness of bulk NiAl at low temperature (< 500 K) are mainly due to limited slip processes. However, a change in deformation behavior takes place with an increase in temperature of NiAl. In the temperature range of 550 K - 700 K, bulk NiAl undergoes a dramatic DBT[3]. The DBTT of 623 K - 673 K and 473 K have also been reported in <100> and <110> oriented bulk single crystals NiAl, respectively[2].

It is also reported experimentally that bulk NiAl and its alloys show a DBTT of 1000 K for single phase single crystal nickel aluminides as well as for directionally solidified two phase Ni-30Al alloys, as reported by Noebe[3], *et al*. The effect of strain rate on the DBT of NiAl bulk alloys has also been reported by many researchers[4-7]. Ebrahimi and Hoyle have shown the effect on DBTT, due to the addition of Ti in NiAl that shows increase in yield strength and DBT temperature. Hence, it may result in an increase in the apparent low temperature toughness[5]. It is reported by Ebrahimi & Hoyle[5], that NiAl shows fracture toughness of ~ 10 MPa.m^{½} (between 27 ^{0}C – 300 ^{0}C) as compared to fracture toughness of ~ 15 MPa.m^{½} – 18 MPa.m^{½} (between 27 ^{0}C – 300 ^{0}C) for NiAl+Ti. It is also shown that a decrease in the applied displacement rate allows the relaxation of internal stresses and decreases the DBT temperature[5]. Effects of temperature and strain rate on the tensile behaviour of multiphase NiAl alloys have also been evaluated experimentally[6]. Cui[6], *et al.* have also reported a DBTT of 1178

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K at a strain rate of $1.04\times10^{-4}\,s^{-1}$ and have shown dependence on the strain rate, with a two order of magnitude increase in strain rate resulting in 120 K increase in DBTT. All the above mentioned studies have been performed on bulk materials with main focus of alloying and effect of strain rate on the DBTT. However, DBT in nano-crystalline NiAl has not been reported in the published literature. In this direction, an attempt has been made to study the effect of orientations on the DBT of NiAl in the form of one dimensional nanowire under uniaxial tensile loading utilizing molecular dynamics (MD) simulations with varying temperature. It is important to mention here that being small in size; experimental validation of such phenomena is a great challenge. However, Seo[7], *et al.* has recently shown large deformation of <110> oriented Au nanowire under tensile loading experimentally. It is an indication that experimental validation of nanoscale phenomena is indeed possible.

In recent past, MD simulations have been used extensively in understanding the structural and thermo-mechanical behaviors of materials at nanoscale[8-11] including effect of free surfaces on the martensitic cubic-to-tetragonal transformation in Ni-Al alloy[12], effect of strain rate and temperature on the mechanical properties of Ni-Al nanowire[13], asymmetry in structural and thermo-mechanical behavior of B2-NiAl nanowire under tensile and compressive loading[14], etc. Recently, it has been observed that an initial <100> oriented B2-NiAl nanowire undergoes B2-BCT phase transformation for a given range of temperature[15-16]. It has also been shown that in the temperature range of 700 K - 900 K, <100> oriented B2-NiAl nanowire shows a very large plastic strain, i.e. of the order of ~700 per cent[17], also known as super-plasticity[18]. It has been observed that <100> oriented B2-NiAl nanowire that shows an abrupt transition in ductility (i.e. increase in failure strain from 35 per cent to ~700 per cent) with an increase in temperature (from 500 K to 700 K). The transition region (~600 K), below which the nanowire shows small ductility and fracture toughness. On the other hand, nanowire shows a large plastic strain (known as superplasticity) before the complete fracture. The region where this separation occurs is considered as ductile-brittle-transition (DBT), as it shows an 'S' shaped curve in toughness - temperature diagram[5] for further details). In the present study, the transition region in an initial <100> oriented B2-NiAl nanowire is identified and reported. Thermo-mechanical responses of other two orientations i.e., <110> and <111> of an initial B2-NiAl nanowire have also been studied under uniaxial tensile loading. The effects of nanowire size, temperature, and orientations on the DBTT have been explored in details.

2. MODELING AND SIMULATION DETAILS

Molecular dynamics (MD) simulations of B2-NiAl nanowire is performed using the embedded atom method (EAM)[19,20]. In the EAM, the total energy U_{total} of a binary system of atoms *A*-*B* is represented as

$$U_{total} = \sum_{i=1}^{N} F_{\alpha_i}\left(\overline{\rho}_i\right) + \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1,\, j\neq i}^{N} \varphi_{\alpha_i-\alpha_j}\left(r_{ij}\right), \qquad (1)$$

where $\varphi_{\alpha_i-\alpha_j}\left(r_{ij}\right)$ is a pair-wise interaction potential as a function of distance r_{ij} between atom *i* and *j* that have chemical sorts α_i and α_j (*A* or *B*), and $F_{\alpha i}$ is the embedding energy of an atom of chemical sort α_i as a function of the host electron density $\overline{\rho}_i$ induced at atom site *i* by all other atoms in the system. The host electron density is given by

$$\overline{\rho}_i = \sum_{j=1,\, j\neq i}^{N} \rho_{\alpha_j}(r_{ij}), \qquad (2)$$

where $\rho_{\alpha_j}(r)$ is the electron density function assigned to an atom of chemical sort α_j. This model involves seven potential functions i.e. $F_A(\overline{\rho})$ and $F_B(\overline{\rho})$ are the embedding energy functions for atom *A* and *B*; $\rho_A(r)$ and $\rho_B(r)$ are electron density functions for atom *A* and *B*; $\phi_{A-A}(r)$, $\phi_{B-B}(r)$, and $\phi_{A-B}(r)$ are pair-wise interaction functions for atom *A*-*A*, *B*-*B*, and *A*-*B* respectively. In the present work, EAM potential of Mishin[21], *et al.* is used. Due to the comparable values of APB energy and inter-branch-Al energy with experimental data, this potential is able to predict the more accurate phase transformation, plastic deformation and fracture properties of B2-NiAl more accurately, especially at high temperature[21].

The B2-NiAl nanowire is created by generating atomic positions as in the bulk, corresponding to the B2 crystal structure with known lattice constant (a_0) of 2.8712 Å. The B2 crystal structure is equivalent to a body-centered-cubic (BCC) lattice with the Ni atoms at the corners of the unit cell and a single Al atom at the body center. Three different orientations are considered in the present study:

(i) nanowire oriented in the <100> directions with {010} and {001} side surfaces, (will be called as <100> hereafter)
(ii) nanowire oriented in the <110> directions with {010} and {011} side surfaces, (will be called as <110> hereafter), and
(iii) nanowire oriented in the <111> directions with {011} and {112} side surfaces (will be called as <111> hereafter).

Three different cross-sectional sizes of the nanowire have been considered, i.e., ~20x20 Å^2, ~25x25 Å^2, and ~30x30Å^2 with ~5000, ~8500, ~13500 number of atoms, respectively for all the three orientations. Further details on the orientation and the cross-sectional size considered in the present study can be seen in Fig. 1.

Initially, a molecular static (MS) simulation has been performed at a temperature of 0 K, to obtain an initial stress free configuration of the B2-NiAl nanowire. The initial relaxed configurations have been obtained via energy minimization of the nanowire, as performed using the conjugate gradient method. The main aim of performing the MS simulation is to get the potential energy details of <100>, <110>, and <111> orientations of nanowire with varying cross sectional size. For this, ~ 2000-32,000 numbers of atoms have been considered. This study will also be helpful to understand the energetic stability of the nanowire with varying orientations.

Next, uniaxial tensile loading of the nanowire has been performed. After the minimization procedure as discussed above, the ends of the nanowire are constrained. The wires are then thermally equilibrated for a given temperature using the Nose-Hoover thermostat[22,23] for 10 ps with a time step of 0.001 ps. Temperature in the range of 10 K-900 K is considered. A uniaxial tensile loading is then applied

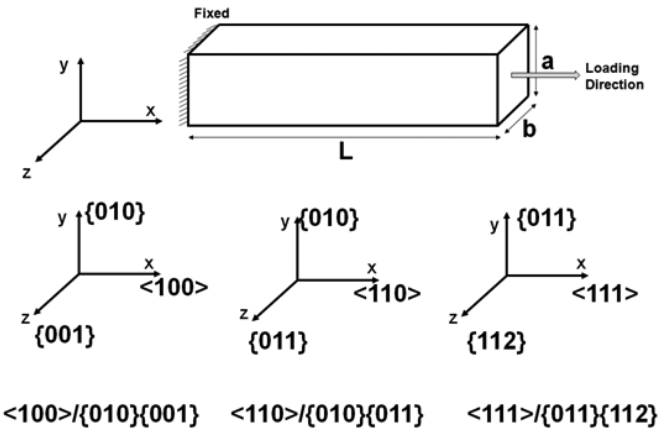


Figure 1. Schematic of the <100>, <110>, and <111> oriented B2-NiAl nanowire and the different side surfaces. (a and b are the cross-sectional sizes and L is the length of the nanowire).

by completely restraining one end of the wire, and then by applying velocity to the atoms along the loading direction, linearly from zero at the fixed end to the maximum value at the free end, thus creating a ramp velocity profile, as shown in Fig. 1. The equations of motion are integrated using velocity Verlet algorithm[24]. Temperature of the system is kept constant during the simulation, which is to capture the isothermal behaviour of the nanowire. The stresses are calculated using the virial theorem[25]. The average virial stress over a volume Ω with total number of atoms *N* is calculated as

$$\Pi = \frac{1}{\Omega}\left(\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1,\, j\neq i}^{N} \mathrm{r}_{ij} \otimes \mathrm{f}_{ij} - \sum_{i=1}^{N} m_i \dot{\mathrm{u}}_i \otimes \dot{\mathrm{u}}_i\right), \qquad (3)$$

where, m_i is the mass of atom *i*. The displacement of atom *i* with respect to the reference position is designated as u_i. $\dot{\mathrm{u}}_i = d\mathrm{u}_i / dt$ represents material time derivative of u_i and $\otimes$ denotes the tensor product of two vectors and $\mathrm{r}_{ij} = \mathrm{r}_j - \mathrm{r}_i$. The force vector **f** can be calculated as $\mathrm{f} = -\frac{\partial U_{total}}{\partial \mathrm{r}_{ij}}$, where, U_{total} is the total potential energy which includes both the pair-wise and many body interactions terms. All simulations are performed using an MD code called LAMMPS[26,27] developed by Sandia National Laboratory. Engineering strain is used as a measure of deformation and defined as $\varepsilon = (l - l_0)/ l_0$, where l is the instantaneous length and l_0 is the initial length of the wire obtained after the energy minimization corresponding to the initial configuration. Toughness is measured by calculating the area under the stress-strain curve. Failure strain ($\varepsilon_f = (l - l_0)/ l_0$) is calculated when the nanowire breaks completely into two parts.

3. EFFECT OF ORIENTATION, SIZE, AND TEMPERATURE ON THE TENSILE STRESS-STRAIN

Figures 2 (a) and 2 (b) show the uniaxial tensile stress-strain behavior of an initial B2-NiAl nanowire at a temperature of 100 K for <100>, <110>, and <111> orientations with varying cross-sectional dimension of 20x20 Å^2 and 30x30 Å^2, respectively. The stress-strain behavior of an initial <100> oriented B2-NiAl shows B2→BCT phase transformation during the tensile loading (see refs [14-15] for further details). It can be seen from the Fig. 2 that an initial <100> oriented B2-NiAl nanowire first shows yielding of the initial B2 phase (marked as A in Fig. 2(a)), afterwards nanowire shows B2-BCT phase transformation followed by the yielding (marked as A' in Fig. 2(a))and fracture of BCT phase. In the case of <110> and <111> oriented nanowire, the nanowire show the yielding of the initial B2 phase (marked as A in Fig. 2 (a)), afterwards formation of necking occurs (marked as B in Fig. 2 (a)), which cause complete fracture of the nanowire without any B2-BCT phase transformation. Figures 2(c) and 2(d) show the uniaxial tensile stress-strain behavior of an initial B2-NiAl nanowire at a temperature of 300K for <100>, <110>, and <111> orientations with varying cross-sectional dimension of 20x20 Å^2 and 30x30 Å^2, respectively.

It can also be seen from the Fig. 2 that the <111> oriented B2-NiAl nanowire shows highest yield stress followed by <110> and <100> oriented nanowire for a given temperature. Further the decrease in the yield stress can be seen with an increase in temperature for all the orientation of the nanowire, as shown in Figs. 2(a) and 2(b) for 100 K and 300 K, respectively. To correlate the variation of yield stress with the orientations, energetic studies have been performed via molecular static (MS) simulations. The details of the initial potential energy before the energy minimization of the nanowire for <100>, <110>, and <111> orientations have been shown in Fig. 3. Results show that with an increase in the number of atoms for a nanowire, the potential energy reduces, as it becomes bulk in nature. It is observed that the <111> oriented nanowire is energetically most stable, whereas the <100> orientation are energetically less stable as compared to the <111> orientation. Results indicate that <111> oriented nanowire, which is energetically more stable leads higher yield stress.

4. DUCTILE-BRITTLE-TRANSITION AND RELATED DISCUSSIONS

4.1 Effect of Nanowire Orientation on DBT

Figures 4(a), 4(b), and 4(c) show percentage failure strain with varying temperature and cross-sectional dimensions of the B2-NiAl nanowire with an initial orientation of <100>, <110>, and <111>, respectively. Results show that all three orientations of B2-NiAl nanowire undergo DBT under uniaxial tensile deformation with an increase in temperature. The results observed for nanowire is also compared with the experimental results of bulk single crystal NiAl[2]. Noebe[3], *et al.* have shown a range of DBTT of 550 K - 700 K in a review of the plastic flow and fracture behavior of NiAl based intermetallic alloys[3] (and the references sited thereof). As the results reported in Noebe[3] *et. al.* are based on a large set of data, we have considered the experimental DBTT of bulk single crystal B2-NiAl in the range of 550 K - 700 K for comparing the present results obtained for NiAl nanowire (Marked as shaded region in Figure 4). DBTT of 623 K – 673 K in <100> oriented single crystals NiAl is reported experimentally[2]. Experimental results also show DBTT around 473 K for the <110> oriented single crystals[2]. It can be seen clearly from the Figs. 4(a), 4(b), and 4(c) that the temperature region where transition in failure strain (DBT) observed in the present study is in similar direction with the

DBT of the experimental values reported by Noebe[3], *et al.*

4.2 Design Aspects for Improving Toughness and DBT

As per the DBT designing point of view, the room temperature (RT) toughness can be improved by shifting the DBTT below RT and/or increasing the lower-shelf toughness level[1], as shown schematically in Fig. 5. The region below the temperature T_1 (line marked as brittle curve) is considered as lower-shelf region, as shown in Fig. 5. This is because of the fact that at lower temperature NiAl has lower toughness due to the limited ductility and hence, leads to a lower shelf region in the toughness – temperature diagram. In polycrystalline form NiAl has a lower-shelf toughness of 10-15 MPa.$m^{1/2}$ and a DBT temperature around 400 °C[1,5]. Figure 5 shows that brittleness of a material can be viewed as a low, lower self toughness or a high, ductile-brittle-transition-temperature (DBTT) as depicted schematically in Fig. 5[1]. The corresponding results obtained for nanowire with varying orientations are shown in Fig. 6.

To see the effect of yield strength on DBT, toughness *vs* temperature has been plotted in Fig. 6. Toughness of the material is calculated from the area under the stress-strain curve. It is known that the yield stress normally reduces with an increase in temperature for a given size and strain rate[15-16] for B2-NiAl nanowire. It is observed that toughness of the nanowire normally decrease with an increase in temperature in the lower shelf region (as shown in Fig. 6(a) and (c) for <100> and <111>

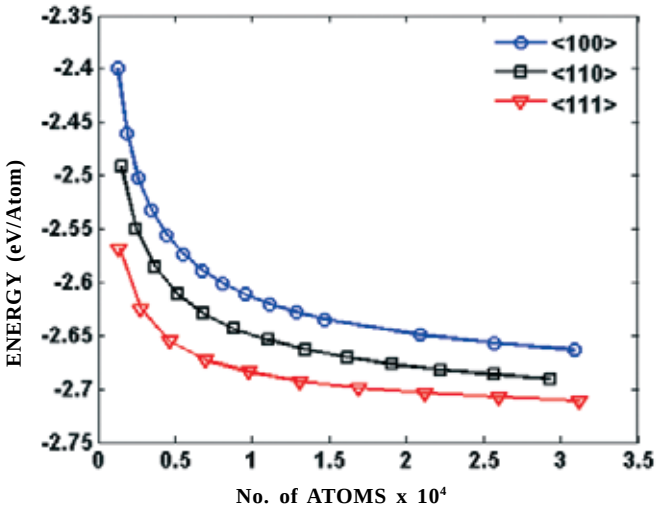


Figure 3. Variations of potential energy of an initial B2-NiAl nanowire with varying size and orientations.

orientation) for temperature up to 600 K [whereas in the case of <110> orientation (see Fig. 6(b)) it's fluctuates)]. This is due to the fact that the yield stress of material reduces with increase in temperature (if a common failure strain of a given material is considered). Above transition temperature, the B2-NiAl nanowire shows transformation from crystalline to amorphous phase after the yielding that causes nanowire to deform more plastically and leads to an increase in toughness.

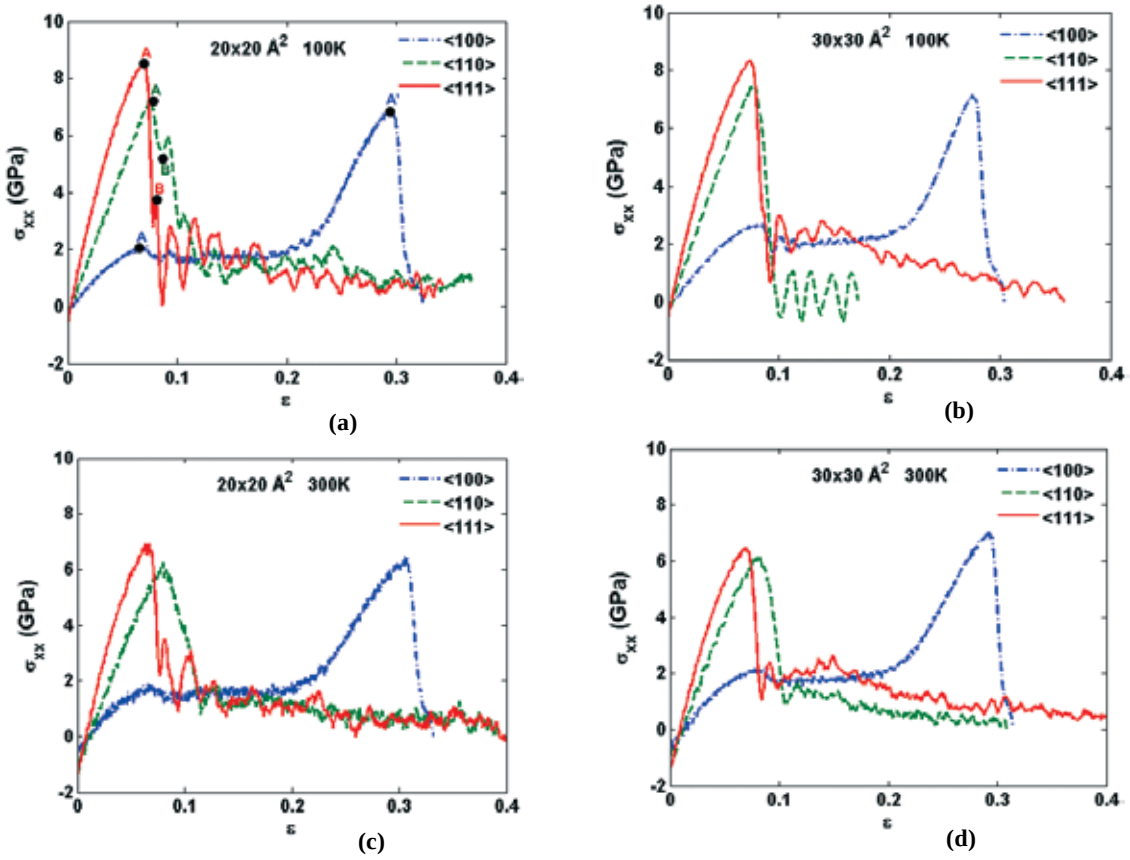
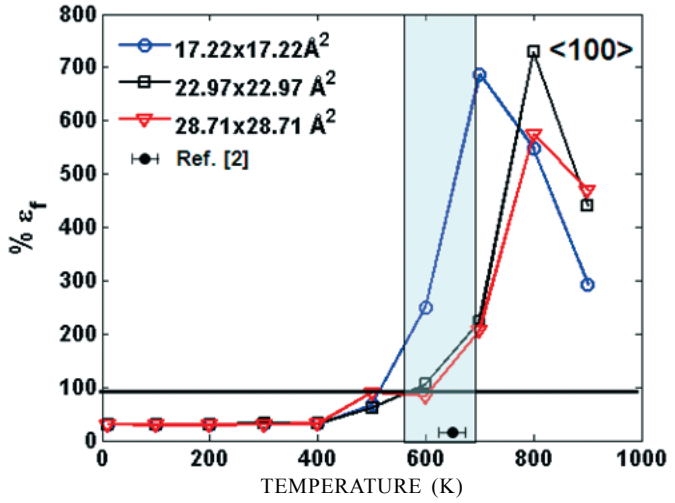
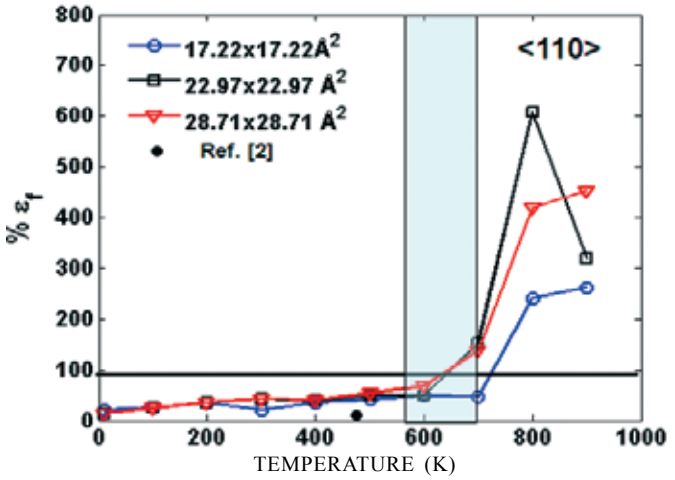


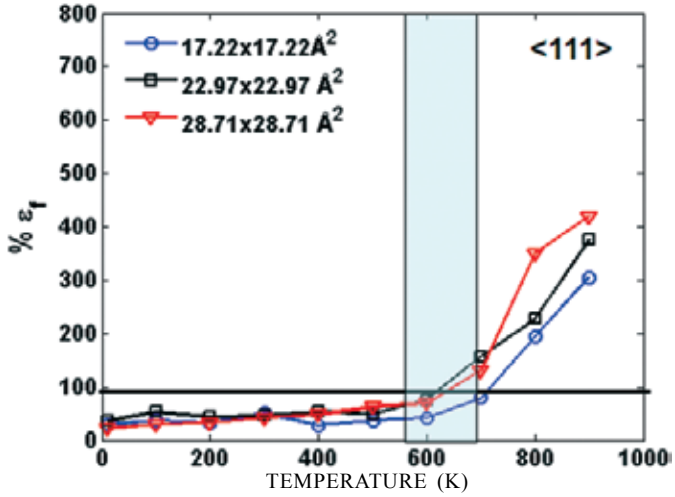
Figure 2. Stress-strain behavior of an initial B2-NiAl nanowire for <100>, <110>, and <111> orientations at a given temperature of 100K and cross-sectional size of (a) 20x20 Å2 and (b) 30x30 Å2; at a temperature of 300K and cross-sectional size of (c) 20x20 Å2 and (d) 30x30 Å2. The yielding and necking is marked as A and B, respectively. The yielding of BCT phase of <100> nanowire is marked as A'.



(a)



(b)



(c)

Figure 4. Percentage Failure strain (% ε_f) of an initial (a) <100>, (b) <110>, and (c) <111> oriented B2-NiAl nanowire with varying temperatures and cross-sectional sizes. The shaded region shows experimental values of DBTT for single crystal B2-NiAl in the range of 550-700K[3].

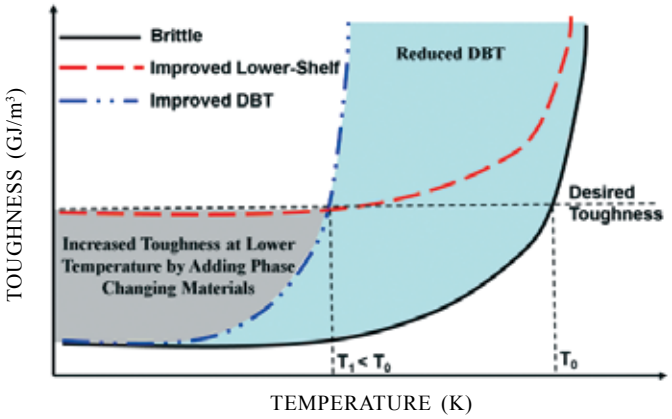


Figure 5. A schematic shows an increase in lower-shelf toughness by adding phase changing material to base alloy material. T_0 is the DBT temperature for the original material and T_1 (< T_0) is the improved DBT.

To minimize the size effect on the DBTT, an overall effect of nanowire orientations on DBT have been studied via comparing the average toughness, as shown in Fig. 6(d). Toughness is calculated by performing average at a given temperature for all the cross-sectional dimensions of nanowire considered for a particular orientation. It can be seen from the Fig. 6(d) that at the lower-shelf region the <100> oriented B2-NiAl nanowire gives higher toughness as compared to other orientations of the nanowire. From the energetic point of view, the <100> oriented nanowire that are the less stable (as shown in Fig. 3) should have lowest toughness as compared to the <110> and <111> oriented nanowire. However, the <100> B2-NiAl nanowire that undergoes B2-BCT phase transformation during the tensile loading leads to the increase in toughness at the lower-shelf region. If we neglect the increase in toughness due to the B2-BCT phase transformation in <100> oriented nanowire, the orientation dependent energy of nanowire can be compared with the toughness at the lower-shelf region. The hypothetical toughness values of <100> nanowire (neglecting the B2-BCT phase transformation is shown as dashed line in Fig. 6(d)). The <111> oriented nanowire that is most stable (energetically) gives highest lower-shelf toughness (after neglecting the B2-BCT phase transformation of <100> nanowire). The procedure followed for calculating the hypothetical toughness is discussed below.

It is well known that the total strain (ε_{Total}) of a stress-strain curve can be written as

$$\varepsilon_{Total} = \varepsilon_{Elastic} + \varepsilon_{Plastic} \tag{4}$$

where $\varepsilon_{Elastic}$ is the elastic strain part and $\varepsilon_{Plastic}$ is the plastic strain part. In the case of <100> B2-NiAl nanowire, the elastic strain part ($\varepsilon_{Elastic}$) can further be decomposed as

$$\varepsilon_{Elastic} = \varepsilon_{B2} + \varepsilon_{PT} + \varepsilon_{BCT} \tag{5}$$

where ε_{B2} is the elastic strain due to the deformation of the initial B2 phase, ε_{PT} is the elastic strain due to the B2-BCT phase transformation, and ε_{BCT} is the elastic strain of BCT phase. If we neglect the phase transformation and related strain part from Eqn. (5), the Eqn. (4) can be written as

$$\varepsilon_{Total}^{*} = \varepsilon_{B2} + \varepsilon_{Plastic} \tag{6}$$

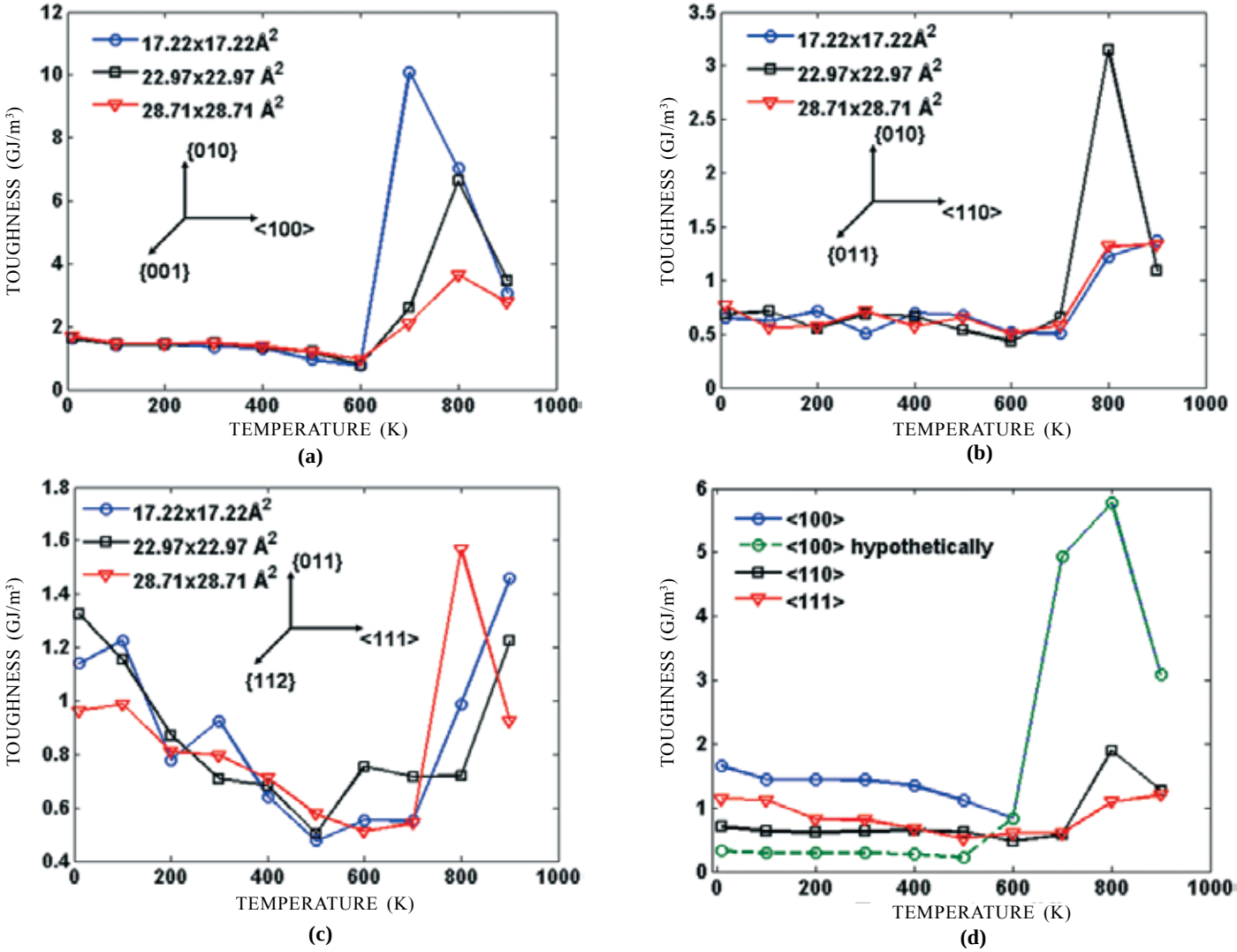


Figure 6. Variations of toughness with varying temperature for (a) <100>, (b) <110>, (c) <111> oriented B2-NiAl nanowire. (d) Average toughness with varying temperature for differently oriented nanowire. (The toughness due to the B2→BCT phase transformation contribution is neglected in the case of <100> hypothetically)

The strain (ε_{Total}^{*}) has been considered for calculating the hypothetical toughness of an initial <100> oriented B2-NiAl nanowire, as shown in Fig. 6(d). Results show that the toughness calculated based on Eqn. (6) is approximately 20% of the total toughness (Eqn. (5)) of actual <100> oriented B2-NiAl nanowire. It is also important to mention here that above 600K similar ε_{Total}^{*} and ε_{Total} is obtained. This is due to the fact that above 600K temperature, no B2-BCT phase transformation is observed in <100> NiAl nanowire. Result indicates that room temperature toughness at lower-shelf region of a given materials could be improved by adding phase changing materials. However, the confirmation of improved toughness at lower-shelf region via experiment and computational design for lowering the DBT is still an open area of research.

5. CONCLUSIONS

An orientation dependent DBT in B2-NiAl nanowire is reported with an increase in temperature. It is found that the <100> B2-NiAl nanowire, which is energetically less stable lead to lower yield stress. Thermo-mechanical properties of nanowire are also explored in details, to find out the design improvements in the room temperature (RT) toughness either by shifting the DBTT below RT and/or increasing the lower-shelf toughness level. Finally, it is proposed that room temperature toughness at lower-shelf region of given materials could be improved by adding phase changing materials. The above suggested techniques needs further verifications from experiments and are still an open area of research.

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