On the Plastic Deformation of a Ni_3Nb Single Crystal*

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The plastic behaviours of a Ni_3Nb single crystal are studied by tensile and compression tests. Three shear systems are found to operate. They are (010)[001] slip, (010)[100] slip and $\{211\}\langle\bar{1}0713\rangle$ twin systems, and the critical resolved shear stresses (CRSS) for these systems are obtained as 44, 51 and 56 MPa in tension, and 55, 64 and 380 MPa in compression, respectively. In case of tensile test, a brittle fracture occurs in almost all the stress orientations, since the CRSS for $\{211\}$ twin in tension is comparatively low and the twin plane is easy to cleave. When the stress axis is parallel to [120], where the twin system is difficult to operate, a ductility can be expected under a tensile test. On the other hand, the CRSS for $\{211\}$ twin in a compression test is considerably high, and the single crystal is plastically deformed up to strains more than 15% by the operation of the (010) slip systems. For the stress orientations parallel to [010] or parallel to the axes on the [100]-[001] great circle, however, the (010) slip systems can not be operated, and it is speculated to be brittle even in a compression test.

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I. Introduction

The intermetallic compound Ni_3Nb , which exhibits a limited ductility, has been considered as a reinforced phase in directionally solidified Ni based eutectic alloys such as $\text{Ni}_3\text{Al}(\gamma')\text{-Ni}_3\text{Nb}(\delta)^{(1)}$, $\text{Ni}(\gamma)\text{-Ni}_3\text{Nb}(\delta)^{(2)}$ and $\text{Ni}(\gamma)/\text{Ni}_3\text{Al}(\gamma')\text{-Ni}_3\text{Nb}(\delta)^{(3)}$. Although it has been found that Ni_3Nb in these eutectic alloys is deformed by means of twin and slip mechanisms, there are few studies of mechanical properties conducted on bulk Ni_3Nb specimens. Studies of the deformation behavior of Ni_3Nb single crystals are, therefore, necessary to reach more complete understanding of the mechanical properties of the above eutectic composites.

Ni_3Nb has an ordered orthorhombic $\beta\text{-Cu}_3\text{Ti}$ type crystal structure⁽⁴⁾, and the growth direction in these eutectic alloys⁽¹⁾⁻⁽³⁾ is [100]. When a tensile stress is applied parallel to the growth direction of the eutectic alloy and the stress reaches the macroyield stress, Ni_3Nb in

the alloy begins to be deformed mainly by $\{211\}$ twin shear. After the twin is generated, (010) slip is observed in or near the twin⁽⁵⁾⁽⁶⁾. This is due probably to the fact that the Schmid factor for the (010) slip system becomes different from zero in the twin. In addition to these two shear systems, the deformation of Ni_3Nb by $\{011\}$ twin has been reported in compression tests on eutectic alloys of $\gamma\text{-}\delta^{(5)(6)}$ and $\gamma/\gamma'\text{-}\delta^{(7)}$. Since the $\{011\}$ twin is usually activated in very high stress conditions compared to the stress for $\{211\}$ twin⁽⁶⁾⁽⁸⁾⁽⁹⁾, it is considered that the main shear systems in Ni_3Nb under tensile stress are $\{211\}$ twin and (010) slip.

The direction of the twin shear on the $\{211\}$ plane is approximately $\langle\bar{1}0713\rangle^{(6)(10)}$, while the shear direction on the (010) slip plane has not been clearly determined. Grossiord *et al.*⁽¹⁰⁾ and Sheffler *et al.*⁽⁷⁾ reported that (010) slip will occur in the close packed direction [100], and dislocations on the (010) with b vector parallel to [001] was observed by Bhowal and Metzger⁽⁸⁾. From measurements of anisotropy in the Knoop hardness of a Ni_3Nb single crystal⁽¹¹⁾, we have speculated that there are four shear systems and that their critical resolved shear stresses (CRSS) increase in the following order: (010)[001], (010)[100], $\{211\}\langle\bar{1}0713\rangle$

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and $\{101\}\langle\bar{1}01\rangle$. In the present work, the CRSS for the operating shear systems in Ni_3Nb are determined from tensile and compression tests of single crystals. The properties of brittleness and plasticity of single crystals are also discussed.

II. Experimental Procedure

Ni_3Nb ingots with a diameter of about 4 mm and containing 75 at%Ni were prepared from 99.9 mass% pure nickel and niobium by induction melting in an alumina crucible under an argon atmosphere. Single crystals 5 mm in diameter and 120 mm long were prepared in high purity alumina crucibles by directional solidification of the ingots. The travelling rate of the specimen was 2.2×10^{-3} mm/s and the temperature gradient was about 8 K/mm. The single crystals were homogenized for 360 ks at 1273 K in an evacuated silica tube. The tensile and compression test specimens were prepared to have several stress axes using a wheel cutter and a discharged machine. After precision shaping with emery papers the specimens were polished with alumina powder, and then annealed at 1173 K for 86.4 ks to remove residual strain. The lattice parameters of the annealed specimen powder were $a=0.5119$ nm, $b=0.4243$ nm and $c=0.4537$ nm.

The tensile tests were performed both at room temperature and at 773 K. The specimens for the tensile test had hangers on both sides, and the dimensions of the gage section were approximately $2 \times 1.5 \times 20$ mm³. The compression tests were done at room temperature using rectangular specimens with dimensions of about $2 \times 2 \times 8$ mm³. Both tests were conducted by a Shimadzu 1S-500 testing machine with crosshead speed of 8.33×10^{-3} mm/s. After straining, the deformation traces on the surface were observed with an optical microscope equipped for Nomarski interference contrast, and the shear planes were analyzed with standard trace analysis. The variations in the axis orientations with the strain were examined by the Laue X-ray technique.

III. Results

1. Tensile tests

The stress-strain curves in tension at 298 K and 773 K are shown in Fig. 1. The axis orientations of the specimens tested in this study are also shown in the figure. Although the single crystals are practically not elongated along either the A or B axis, traces of plastic deformation are observed on the surfaces of all test pieces, and specimen B showed slightly larger strain than specimen A. These tensile behaviors are practically unchanged between 298 and 773 K.

Figure 2 shows the surface of specimen B fractured in tension at 298 K. Fine traces of (010) slip are observed uniformly over the whole surface of the gage section. A small amount of $\{211\}$ twin is observed only near the fracture surface. Figure 3 is a SEM micrograph of the fracture surface composed of four $\{211\}$ planes. From the fractography, it is assumed that the fracture of specimen B occurred by cleavage on the $\{211\}$ twin plane. In specimen A, traces of $\{211\}$ twin were numerous at or near the fracture surface but there were no traces of (010) slip. Specimen A also fractured

Fig. 1 Stress-strain curves of Ni_3Nb single crystals in tension at 298 K and 773 K.

Fig. 2 Deformation traces observed on the surface of specimen B tested in tension at 298 K.

Fig. 3 Fracture surface of specimen B tested in tension at 298 K.

by cleavage on the $\{211\}$ crystal plane.

The $\{211\}$ twin was always present at the fracture portion, and the fracture surface consists of the $\{211\}$ crystal plane, independent of the tensile axis. It is concluded from the tensile tests that the stress required to operate the $\{211\}$ twin is low and the twin plane is easy to cleave. Because the Schmid factors of the specimen A for (010) slip and $\{211\}$ twin under the applied stress along $[100]$ direction are 0 and 0.47, respectively, the $\{211\}$ twin may operate but the (010) slip does not occur. Once the twin operates in the specimen A, the cleavage fracture progresses and the specimen shows no plasticity. As shown in Fig. 1, it is obvious that specimen B, which is oriented approximately in $[331]$, shows a larger plastic strain than A. This larger strain is due to the operation of (010) slip prior to the cleavage fracture.

2. Compression tests

The effects of the stress axis on the stress-strain curves in compression at room temperature are illustrated in Fig. 4. As compared with the tensile test, the orientation dependence of the plasticity in compression is remarkable. Specimens B, C and D showed significant amounts of plastic strain more than 15%. On the other hand, specimen A buckled or crushed into pieces without any visible plastic strain. However, the stress of buckling or crushing (about 800 MPa) was considerably higher than the fracture stress obtained from the tensile test for the specimen A (100–150 MPa).

The deformation traces on the surface of specimen A tested in compression are shown in Fig. 5. All traces correspond to the four $\{211\}$ twins. A large number of the twins occur all over the test piece, but the total amount of plastic strain is rather small as can be judged from a narrow width of each twin. Figure 6

Fig. 4 Stress-strain curves of Ni_3Nb single crystals in compression at 298 K.

Fig. 5 $\{211\}$ twins observed on the surface of specimen A tested in compression at 298 K.

Fig. 6 (010) slip traces observed on the surface of specimen B tested in compression at 298 K.

shows fine traces of plastic strain on specimen B, and the traces reveal the operation of slip on the (010) plane. On the surfaces of specimens C and D, (010) traces similar to the specimen B were observed.

The compression tests show that the Ni_3Nb single crystal is deformed plastically only when the (010) slip operates, while it is brittle once the $\{211\}$ twin occurs, in a similar way to the results of the tensile test. The shear directions of the (010) slip determined from the variation in the axis orientation with the compression strain were $[100]$ for specimen B and $[001]$ for specimen D. The latter had a stress orientation of about $[122]$ prior to the deformation. The shear direction of specimen C, in which the initial orientation is nearly $[111]$, could not be determined.

3. Shear stresses

The results at room temperature are summarized in Table 1 which shows the yielded stress (σ) and CRSS (τ) for a primary shear

system along with stress axis and the Schmid factor. The CRSS for the $\{211\}$ twin were determined from the cleavage stress in tension and the buckling or crushing stress in compression for specimen A, the shear direction of the $\{211\}$ twin being treated as $\langle \bar{1}0\ 7\ 13 \rangle$ in accordance with Grossiord *et al.*⁽⁶⁾⁽¹⁰⁾. The stress to operate the $(010)[100]$ slip system in tension was obtained from the 0.2% flow stress for specimen B. The CRSS in compression for the $(010)[100]$ and $(010)[001]$ slip systems were calculated at 0.2% flow stress for specimens B and D. The yield and shear stresses for the shear systems which did not operate are also shown in parentheses. The shear stress for the $\{211\}$ twin obtained from specimen A is 56 MPa in tension and 376 MPa in compression, and the stresses to operate a $\{211\}$ twin in specimens B, C and D were estimated at about 200, 180 and 170 MPa in tension, and at about 1400, 1200 and 1100 MPa in compression. In the compression test, the CRSS for the $(010)[001]$ slip is 55 MPa and is 0.86 times as high as

Table 1 Shear system, Schmid factor, yield stress and critical resolved shear stress. (): calculated value, *: slip direction is not clear.

Stress axis	Shear system	Schmid factor	Tension		Compression	
			σ_y (MPa)	τ (MPa)	σ_y (MPa)	τ (MPa)
A [100]	$\{211\}\langle\bar{1}0713\rangle$	0.47	120	56	800	376
	(010)[001]	0				
	(010)[100]	0				
B ~[331]	$(21\bar{1})[10\bar{7}13]$	0.27	(207)		(1393)	
	(010)[001]	0.20				
	(010)[100]	0.46	110	51	140	64
C ~[111]	$(21\bar{1})[10\bar{7}13]$	0.31	(181)		(1213)	
	(010)[001]	0.28				56*
	(010)[100]	0.32			200	64*
D ~[122]	$(211)[10\bar{7}13]$	0.33	(170)		(1139)	
	(010)[001]	0.39		(44)	140	55
	(010)[100]	0.28				

that (64 MPa) for (010)[100] slip. The same ratio is applied to the case of tensile test, and 44 MPa is obtained for the stress to operate (010)[001] slip (D axis), since the stress for (010)[100] of B stress axis in tension is 51 MPa.

IV. Discussion

The authors⁽¹¹⁾ have previously studied the shear systems of Ni_3Nb through measurements of anisotropy in Knoop hardness. The operating shear systems revealed in the present study are the following three systems; (010)[001] slip, (010)[100] slip and $\{211\}\langle\bar{1}0713\rangle$ twin. The order of magnitude of the CRSS obtained for these systems nearly coincides with the order suggested by the study on hardness anisotropy. The $\{101\}\langle\bar{1}01\rangle$ system, which was not observed here, is considered to operate under particular stress conditions such as those in hardness measurements.

It is shown that the Ni_3Nb single crystals which have been considered brittle can be deformed plastically in compression, depending on the axis orientation, even at room temperature. Quinn *et al.*⁽²⁾ measured the effects of temperature on the hardness of Ni_3Nb and obtained about 70 H_R between 293 and 1000 K, independent of the test temperature. The tensile behavior at 773 K is almost identical to that at room temperature

(Fig. 1). Therefore, it can be said that the orientation dependence of the plastic behavior of Ni_3Nb single crystal is practically unaltered in this temperature range. The present experimental results show that the effects of orientation on the deformation behavior depend not on the test mode (tension or compression), but on the operation of the $\{211\}$ twin. It is considered that whether a Ni_3Nb single crystal behaves as a ductile or a brittle one is controlled by the relative magnitude of the CRSS for each shear systems and the Schmid factors.

Figure 7 shows the equi-Schmid factor lines for the (010)[100] and (010)[001] slip systems. The signs from A to D in the figure are the initial axis orientations of the specimens used. On the thick broken line in the figure, the Schmid factor for [100] is equivalent to that for [001]. Since the shear stress for (010)[100] is slightly larger than that for (010)[001] (Table 1), the axis orientations where the resolved stresses of both slip systems are equal are located slightly below the broken line, where the Schmid factor ratio of (010)[100] to (010)[001] is 1.16. It can be understood from Fig. 7 that the axis orientation A can not operate (010) slip system, and the axis orientations B and D are convenient to operate (010)[100] and (010)[001] slip system, respectively. As is understood from the Schmid factor ratio, 1.14, for both the slip systems along the C

Fig. 7 Equi-Schmid factor lines for the (010)[100] and (010)[001] slip systems.

orientation, the resolved stresses for the two systems in the specimen C are almost identical and CRSS for both systems almost coincide with the stress determined from the specimens B and D (Table 1). This suggests the possibility to operate both the slip systems in the specimen C, and this may be the reason why the shear direction could not be determined with the specimen C. In either the [100] or [001] slip direction, however, the slip on the (010) plane shows ductility.

Although the $\{211\}$ twin shear system operates in specimen A, where the (010) slip can not operate, the plastic strain is negligibly small, and once the $\{211\}$ twin occurs, the specimen breaks in both the tension and compression tests. The brittleness is particularly pronounced in tension, because the tensile shear stress for the twin is very low and the specimen is easily cleaved at the twin plane. For example, along the B axis orientation, where the specimen showed a ductility in compression, there is no plasticity in tension due to cleavage arising from the twin operation. Under tensile tests, the stress required to operate the $\{211\}$ twin in specimen B is as low as 200 MPa, and this stress is easily reached after the yield by the (010) slip. The specimen B can be deformed plastically in compression, because the compressive stress to operate the

Fig. 8 Equi-Schmid factor lines for the four $\{211\}\langle 10\bar{7}13\rangle$ twin systems.

twin is higher than 1400 MPa and the stress for the (010) slip does not exceed this value even in the stage of work hardening. This also explains the ductility of specimens C and D under compression. A stress higher than 1000 MPa is required to operate the twin in these specimens.

The shear stress for the $\{211\}$ twin is high in compression and low in tension, and it can be generally said that a Ni_3Nb single crystal is brittle under a tensile stress and ductile under a compressive stress. Depending on the axis orientation, however, there will be cases where the single crystal behaves occasionally as a ductile one even in tension. Figure 8 show the equi-Schmid factor lines for the four $\{211\}$ twin systems. For an axis orientation around [120], a stress higher than 500 MPa is necessary to operate the twin system in tension. The Schmid factor for (010)[100] around the [120] axis is higher than 0.4, and it is possible to operate the (010)[100] slip by a tensile stress lower than 110 MPa. Therefore, if the axis orientation is at or around [120], plastic deformation can be expected even in tension without the occurrence of the $\{211\}$ twin. On the other hand, the slip on (010) plane can not operate by the stress oriented parallel to [010] or parallel to one of axes on the [100]-[001] great circle, and specimens with these orientations are speculated to be brittle even under compression stress as specimen A is.

V. Conclusion

The shear systems to operate in the Ni_3Nb single crystal and their CRSS were studied by tensile and compression tests. It has become clear that the crystal can be deformed plastically if the shear by the $\{211\}$ twin mechanism does not work. The results may be summarized as follows:

(1) There are three shear systems to operate, the $(010)[001]$ slip, the $(010)[100]$ slip and the $\{211\}\langle\bar{1}0\ 7\ 13\rangle$ twin; their CRSS were obtained as 44, 51 and 56 MPa under tensile stress, and 55, 64 and 380 MPa in compression, respectively.

(2) In the tensile test, a brittle fracture occurred in almost all the stress orientations, since the CRSS for the $\{211\}$ twin in tension is comparatively low and the twin plane cleaves easily. When the stress axis is parallel to $[120]$, ductility can be expected under a tensile test, because at this stress orientation the twin system is difficult to operate.

(3) In the case of compression tests, the CRSS for the $\{211\}$ twin is quite high, and the single crystal is plastically deformed up to

strains more than 15% by the operation of the (010) slip system. For the stress orientation parallel to the $[010]$ or parallel to the axes on the $[100]$ - $[001]$ great circle, however, the (010) slip systems can not operate and the crystal breaks fragilely.

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