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Microprocesses of the deformation of NiAl single crystals

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Abstract

NiAl single crystals were deformed in soft orientations inside a high-voltage electron microscope. At room temperature, dislocations with ⟨100⟩ Burgers vectors move on {100}, {110} and {210} planes and bow out between jogs. The shape of the bowing is determined by anisotropic line tension. The local effective stress calculated from the bowing is somewhat smaller than the resolved shear stress quoted in the literature. Viscous motion between the stable positions hints at the additional action of the Peierls mechanism. Above about 400°C, the dislocation motion is smooth. It is suggested that it is controlled by diffusion processes. © 1997 Elsevier Science S.A.

Keywords: Dislocation motion; NiAl; In situ straining; Transmission electron microscopy; Effective stress; Flow stress

1. Introduction

NiAl with the B2 structure is a prospective material with a good oxidation resistance for applications at intermediate temperatures. The shortest Burgers vector is of ⟨100⟩ type which does not yield five independent slip systems. At high temperatures, also dislocations with ⟨110⟩ and ⟨111⟩ Burgers vectors are observed. Deformation tests with orientations of the tensile or compression axis away from ⟨100⟩, which are called soft orientations, activate dislocations with ⟨100⟩ Burgers vectors. Inspite of a number of respective studies [1], the mechanisms controlling the dislocation motion and the flow stress are not yet clear. The different Peierls stresses of the different slip systems certainly explain the preference of the ⟨100⟩ Burgers vectors, as suggested by recent calculations [2], but it is open to discussion whether, or not, the Peierls mechanism controls also the deformation in the soft orientations, as originally proposed in [3]. Other mechanisms like the formation of dislocation loops and debris may be important, too [4]. In situ straining experiments in a high-voltage electron microscope have been performed to help elucidate the deformation processes in NiAl as they enable the direct observation of dislocations under load as well as their motion.

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2. Experimental

Micro-tensile specimens were prepared from nominally stoichiometric NiAl single crystals by a two-step electrolytic jet polishing procedure described in [5]. They were fixed to the grips of in situ straining devices for the high-voltage electron microscope for deformation at room temperature [6] or at high temperatures [7]. The samples had (110) foil surfaces and approximately $[1\bar{1}1]$ or $[2\bar{2}1]$ tensile directions. The microscope was operated at 1000 kV. The samples were loaded in small load increments. The dislocation structures were recorded under load on photographic film or on video tape. Usually $[\bar{1}10]$, $[1\bar{1}1]$ or [002] $\vec{g}$ vectors were chosen close to the tensile direction so that all or most of the dislocations with an appreciable orientation factor should be in contrast.

3. Results

Fig. 1 shows the characteristic shape of dislocations with Burgers vectors $b = \langle 100 \rangle$ under load at room temperature. The activated slip planes are identified from slip traces, from emergence points of dislocations through the surface and from the path of the emergence points during motion, recorded on video tape. According to that, the dislocations glide on {100}, {110} and

{210} planes, with frequent cross slip between these planes. The dislocation mobility does not differ very much between the different planes.

Screw dislocations are strongly pinned. The average distance between the pinning agents measured for about 900 segments amounts to $\bar{l} = 76$ nm corresponding to about 260 b, where $b = 0.288$ nm. Between the pinning centres, the bowed-out segments are of angular shape. The main features of this shape can be explained in terms of the line tension model in anisotropic elasticity. Fig. 2 shows the equilibrium shape of loops on {100} and {110} planes, calculated by using elastic constants from Fig. 6 in [1]. As already pointed out in [8], screw dislocations with $b = \langle 100 \rangle$ are unstable on {100} planes. Fig. 2 shows that they are unstable on {110} planes, too. This instability leads to the sharp 'knee' at the screw parts and to a preference of mixed dislocations as in Fig. 1. The local effective shear stress can be estimated from the size of the calculated loops fitting the images of bowed-out dislocation segments. The average value of the minor half axis x_o of the loops, taken from 39 relatively long bowed-out segments, is 95 nm. This value has to be considered a rough estimate because of the angular shape of the segments.

A detailed analysis of the video recordings enabled the obstacles impeding the motion of screw dislocations to be identified as jogs. This is demonstrated in the video sequence of Fig. 3a–i. The dislocation moves on a {210} plane as indicated by the (vertical) [$\bar{1}$12] trail on

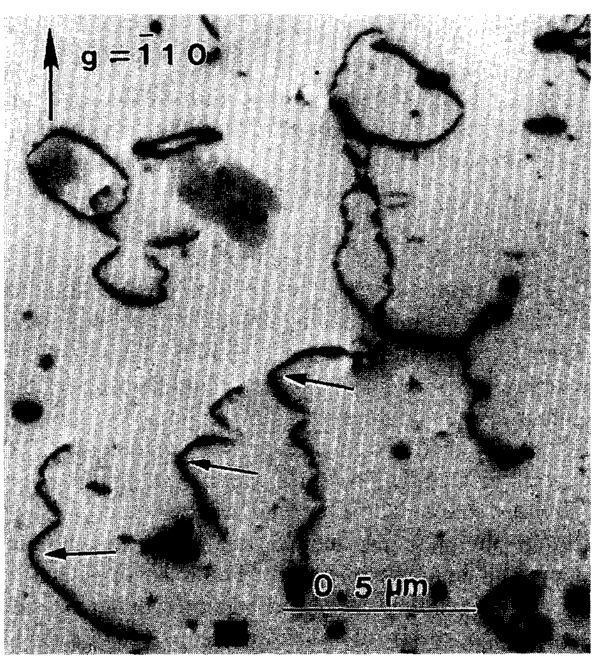

Fig. 1. Dislocations with $b = \langle 100 \rangle$ on {100} planes taken during in situ straining of an NiAl single crystal at room temperature. The projection of b is approximately parallel to g.

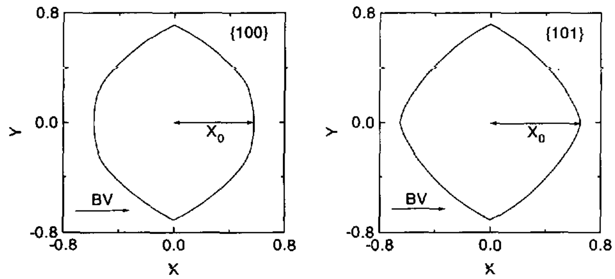

Fig. 2. Shape of dislocation loops with $b = \langle 010 \rangle$ on the {100} and {101} planes calculated by the line tension model in anisotropic elasticity using the elastic constants for room temperature from Fig. 6 in [1].

a (110) plane. The major positions are summarized in Fig. 3j. In (a), a dislocation is anchored by two jogs, J_1 and J_2. Because of the great length of the central segment, the jogs are subjected to an outward tangential force, which leads to a left-shift of J_1 between (a) and (b). In (c) the central segment bows out extraordinarily wide, most probably leading to the creation of debris D in (d). In this frame, two positions of the left part of the dislocation appear in weak contrast due to a quick motion without the jog. Thereby, the dislocation acquired a new jog J_3 by cross slip. It is clearly visible in (f), and is shifted along the dislocation in Burgers vector direction between (f) and (g). The dislocation produces a further debris D at J_2, which causes J_2 to be eliminated and the right part of the dislocation to quickly move between (g) and (h) with a larger width of the slip trail, indicated by thin lines in (j). Finally, between (h) and (i) the right segment moves out of the foil by further cross slip. The most prominent feature of this kind of motion is the formation of long segments by the sideward spreading of the limiting jogs leading to very large bow-outs as in Fig. 3c and labelled by arrows in Fig. 1. These large bow-outs cannot be explained by the action of localized obstacles like precipitates, which is the usual interpretation of curly dislocation shapes. In a precipitation hardening mechanism, after surmounting one obstacle the moving dislocation segment has a large probability to contact a new obstacle after sweeping an area of the order of $\bar{l}^2$ (the small black rectangle at the lower edge of Fig. 1), which usually does not yield a large bow-out. Thus, the formation of many large bow-outs and the sideward spreading of the pinning agents suggest that jogs cause the pinning of screw dislocations in NiAl, in accordance with the cross slip frequently observed. Between the stable positions the dislocations mostly move in a viscous way at a velocity that can be resolved by video recording. This suggests that a lattice friction mechanism is also active, in agreement with the fact that the segments bowed-out under load do not remarkably relax when the specimen is unloaded.

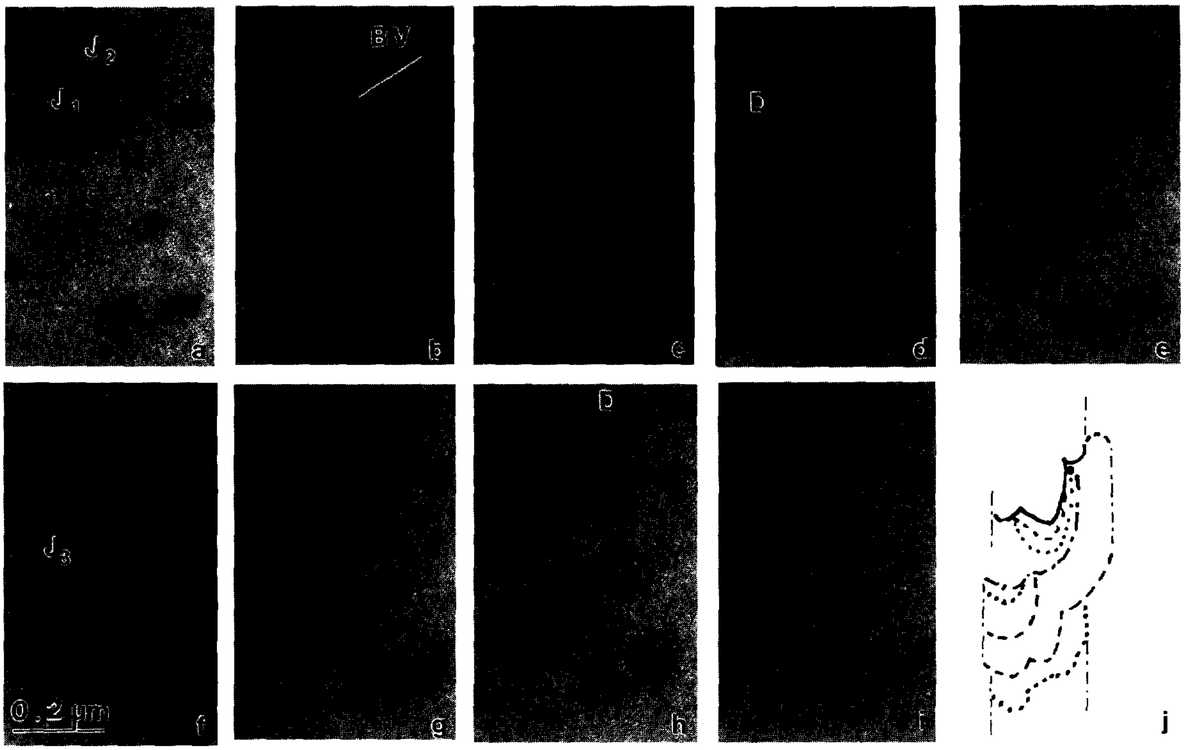

Fig. 3. Sections of a video sequence of the motion of a screw dislocation on a {210} plane at room temperature. Foil plane (110), vertical slip trace [$\bar{1}$12].

High-temperature in situ straining experiments were carried out at about 380, 475 and 565°C. Fig. 4 shows sections of a video recording of the experiment at 475°C. The main features are typical also of the other high-temperature experiments, including a much lower density of jogs compared to room temperature and a viscous motion of the dislocations. The shape of the dislocations predetermined by the anisotropic line tension is still preserved. The average size of the fitting theoretical loops amounts to about $x_0 = 560$ nm. At 475°C slip appears preferentially still on {100} and {110} slip planes with frequent cross slip between these planes. The dislocation marked by arrows changes from a {100} plane in Fig. 4a to a {110} plane in Fig. 4b. At higher temperatures, the slip trails become non-crystallographic so that probably climb, too, contributes to the dislocation motion.

4. Discussion

The present experiments clearly prove that slip of dislocations with ⟨100⟩ Burgers vectors in NiAl appears on {100}, {110} and {210} planes with about equal mobilities, as already discussed in [10] for the {100} and {110} planes. Although {210} slip planes had been found in [9], these planes have not further been discussed in other papers. Frequent cross slip beween the different planes results in the formation of high jogs at room temperature. Between them, the dislocations bow out. According to the line tension theory in anisotropic elasticity, the size of the theoretical loops fitting the bow-outs, represented by their minor half axis x_0, is a measure of the local effective stress τ^* according to

$$\tau^* = E_0/(bx_0)\ \ln(\bar{l}/[5b]), \tag{1}$$

where E_0 ($= 5.8 \times 10^{-16}$ N for room temperature) is the prelogarithmic energy factor of an edge dislocation. With the experimental data above, τ^* becomes about 90 MPa for room temperature, and 20 MPa for 475°C. The stress at room temperature is slightly smaller than the macroscopic yield stress (approximately 200 MPa [3,10]) resolved to the respective glide planes. Thus, the jog mechanism may explain a great part of the macroscopic flow stress. The observed jog distance of $\bar{l} \cong 260$ b should then correspond to the activation volumes measured in macroscopic tests. The data in [11] correspond to very large activation volumes, whereas small values in the order of $10b^3$ are reported in [3]. The latter data are not in accordance with the present obstacle distance but, in connection with the strong increase of the flow stress below room temperature, they suggest the action of the Peierls mechanism. The

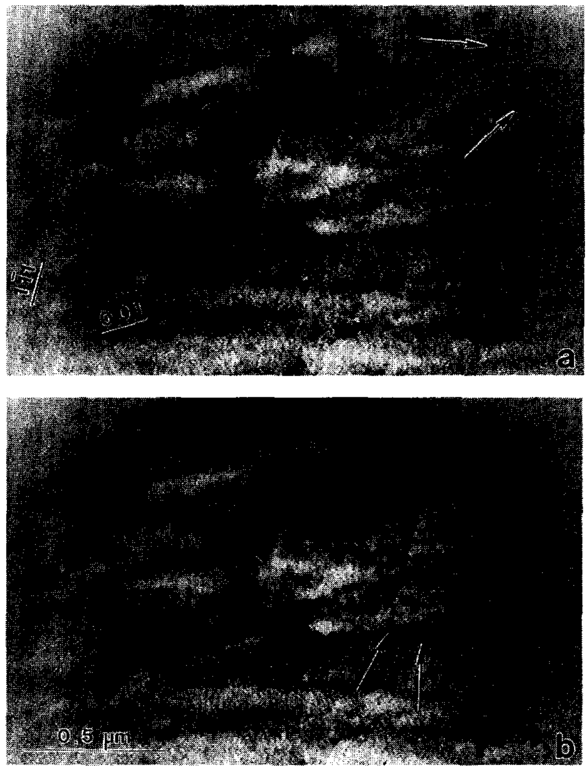

Fig. 4. Video recording of dislocation motion on a {100} plane and cross slip to a {110} plane at about 475°C.

present experiments also hint at a contribution of the Peierls stress, in addition to the jog mechanism, by the viscous motion of the dislocations between the stable positions at jogs and by the fact that the dislocation configurations do not relax after unloading. These present results only partly confirm the theoretical calculations of the Peierls stress in NiAl [2]. As a conclusion, the room temperature flow stress of NiAl is certainly controlled by a jog mechanism together with the Peierls stress, which strongly increases with decreasing temperature.

At the elevated temperature of 475°C, the effective stress $\tau^* \cong 20$ MPa measured from the dislocation bowing is only about 20% of the macroscopic flow stress. Viscous motion of dislocations at these temperatures had already been observed in TiAl [12]. This is a remarkable phenomenon, which cannot be explained by the Peierls mechanism with the data of the low-temperature increase of the flow stress. According to standard theory, thermally activated processes controlling the dislocation mobility at low temperatures should not be active above specific temperatures. Apparently, a new thermally activated process very effectively limits the dislocation mobility at elevated temperatures, which should be associated with lattice diffusion. At high temperatures, climb is indicated by non-crystallographic slip trails. Because of the low mobility of vacancies, characterized by a migration enthalpy of 2.1 eV [13], diffusion processes may become evident only in the temperature range of the viscous dislocation motion and control it. For FeAl [14], a close connection has been observed between the kinetics of vacancy migration, internal friction and the time dependence of the yield stress anomaly so that these diffusion-controlled processes might be considered a more general phenomenon of dislocation motion in intermetallics at elevated temperatures.

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References

[1] D.B. Miracle, Acta Metall. Mater. 41 (1993) 649.
[2] R. Schroll, P. Gumbsch, V. Vitek, Mater. Sci. Eng. A (1997) in press.
[3] R.T. Pascoe, C.W.A. Newey, Metal Sci. J. 5 (1971) 50.
[4] A. Ball, R.E. Smallman, Acta Metall. 14 (1966) 1349.
[5] U. Messerschmidt, In: T. Robarts, A.J. Wilson (Eds.), Procedures in Electron Microscopy, Wiley, Chichester, 1993, Ch. 9.12.
[6] U. Messerschmidt, F. Appel, Ultramicroscopy 1 (1976) 223.
[7] U. Messerschmidt, M. Bartsch, Ultramicroscopy 56 (1994) 163.
[8] M.H. Loretto, R.J. Wasilewski, Philos. Mag. 23 (1971) 1311.
[9] A. Ball, R.E. Smallman, Acta Metall. 14 (1966) 1517.
[10] R.D. Field, D.F. Lahrman, R. Dariola, Mat. Res. Soc. Proc. 213 (1991) 255.
[11] R.J. Wasilewski, S.R. Butler, J.E. Hanlon, Trans. AIME 239 (1967) 1357.
[12] D. Häußler, M. Bartsch, U. Messerschmidt, M. Aindow, I.P. Jones, Institute of Physics Conference Series No. 147, Section 11, IOP, 1995, 463.
[13] H.-E. Schaefer, K. Badura-Gergen, Defects Diffusion Forum 143–147 (1997) 193.
[14] H.-E. Schaefer, B. Damson, M. Weller, E. Arzt, E.P. George, Phys. Status Solidi A 160 (1997) 541.