MICROMECHANISM OF CLEAVAGE FRACTURE IN FERRITIC STEELS

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Metallographic and fractographic analysis of ferritic specimens subjected to mechanical tests in the transition region proved that deformation twinning is an integral part of plastic deformation in the moving crack tip region at transition and sub-transition temperatures. Cleavage microcracks, acting as inherent nuclei of cleavage, initiate on the intersections of active slip bands with unfavorably oriented twins ahead of the approaching crack tip. These pre-cleavage microcracks (PCMC) grow towards the approaching main crack. Thus, the actual fracture mode of ferritic steel is governed by the extent of twinning in the plastically strained volume, i.e. by the size and spacing of the twins.

K e y w o r d s: ductile-to-brittle transition, cleavage fracture, deformation twins, ferritic steel, pre-cleavage microcrack

MIKROMECHANIZMUS ŠTIEPNEHO LOMU FERITICKÝCH OCELÍ

Metalografická a fraktografická analýza feritických vzoriek po mechanických skúškach pri tranzitných teplotách ukázala, že deformačné dvojčatenie je integrálnou súčasťou procesu plastickej deformácie v okolí pohybujúceho sa koreňa magistrálnej trhliny pri tranzitných a subtranzitných teplotách. Štiepne mikrotrhliny, pôsobiace ako inherentné zárodky štiepneho porušenia, iniciujú na priesečníkoch aktívnych sklzových systémov s nepriaznivo orientovanými deformačnými dvojčatami pred čelom rastúcej magistrálnej trhliny. Tieto zárodky (pre-cleavage microcracks, PCMC) rastú smerom k čelu približujúcej sa magistrálnej trhliny. Aktuálny mechanizmus lomu teda závisí od rozsahu deformačného dvojčatenia v plasticky deformovanej oblasti pred koreňom magistrálnej trhliny, t.j. od veľkosti a vzájomnej vzdialenosti deformačných dvojčiat.

1. Introduction – current problems of understanding the ductile-to-brittle transition and cleavage fracture of ferritic steels

Ductile-to-brittle transition (DBT) has been known for more than a century as a phenomenon limiting the exploitation of ferritic steels at low temperatures and

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high strain rates. Over the years the main role of the microstructure and its grain size in controlling DBT has been proved. Despite the extensive research effort the following topics are still a subject for discussion:

– Which basic factors determine the temperature and shape of DBT [1]?

– Is the cleavage propagation-controlled or nucleation-controlled [2]?

– What is the origin of inherent nuclei of cleavage microcracks with size of several μm, indicated by calculations from experimentally measured values of fracture stresses [2]?

Most probably the crack extension from notch or pre-crack on the microscopic level is not a continuous process, but rather a microcrack must first be nucleated ahead of the notch or pre-crack [3]. This microcrack is then loaded by the stress field of the notch or pre-crack and the attendant plastic zone. Nowadays, it is believed that cleavage in ferritic steel most probably initiates in a brittle secondary particle, fractured in the stress field of a pile-up of dislocations [e.g. 2, 4]. The problem of the cleavage fracture of ferritic steel would be thus a problem of the brittle microcrack moving through the nucleating elastic particle and trying to penetrate the deformable matrix [3]. A serious problem is however introduced by the intrinsic tendency of ferritic materials to blunt the tip of existing nuclei through emission or absorption of dislocations.

Though the brittle cementite particles in ferritic steels can be regarded as inherently cracked, ferritic materials undergo DBT even with the carbon content reduced to a level such that particles of 1 μm and more do not exist [2]. Thus it has to be admitted, that some other intrinsic phenomenon occurring in the transition region of ferritic steels might play an important role in initiation of cleavage fracture.

Deformation twins have been known to play an important role in brittle fracture at cryogenic temperatures since the works of Hull [5, 6], who reported a cleavage crack initiation in silicon iron single crystals at -196 ℃ on the intersection of growing twins and proposed the same mechanism also for polycrystalline silicon iron at temperatures of -196 ℃ and -253 ℃. Also, according to Griffiths and Owen [7], cleavage at these temperatures is twin nucleated, whereas at higher temperatures slip nucleated cleavage takes place.

In 1981 Reid [8] reviewed many experiments, linking the occurrence of brittle fracture in bcc metals to deformation twinning, and he concluded, that no conclusive evidence showing both spatial and temporal association was available. A more recent review paper [9] on deformation twinning also concludes, that there is a good evidence that blocked twins can nucleate microcracks in some materials, but incomplete evidence that these cracks may initiate a macroscopic failure. It follows, that even if the possible participation of twinning at cleavage is generally admitted at very low temperatures, they are not supposed to play any significant role in DBT temperature region of structural materials.

However, deformation twinning in bcc metals exhibits several important features, which might support its possible role in DBT and cleavage of bcc metals. Unlike the fcc metals [10], deformation twinning in bcc metals occurs at the very early stages of plastic deformation by slip of dislocations. In fcc metals rather extensive plastic deformation by slip of dislocation usually precedes the twinning. Furthermore, twin bands in bcc metals are usually broad, several micrometers in thickness, while those in fcc metals consist of thin lamellae. The intersections of twin bands or the termination of twin growth at obstacles often cause crack initiation in bcc metals, but not in fcc metals. The twinning direction in bcc crystals has the same orientation as the slip direction, while in fcc metals no such relation exists. It is also important that the stacking fault energy in bcc metals exceeds significantly that of fcc metals. Specific features of deformation twinning in bcc materials can be mainly associated with the restricted possibilities of easy slip before and during twinning in comparison with fcc materials.

The results presented below indicate that deformation twinning most probably plays a dominant role in DBT and cleavage of ferritic structural steels. Deformation twinning was found to be an integral part of plastic deformation in the moving crack tip region at transition and sub-transition temperatures. The intersections of active slip bands with unfavorably oriented twins ahead the moving crack tip acted as initiation sites for cleavage microcracks. These microcracks, growing towards the approaching main crack tip, can be most probably regarded as inherent nuclei of cleavage in ferritic steels, predicted by the theory of brittle fracture.

2. Experimental

2.1 Materials and procedures

Ductile to brittle transition properties of several ferritic materials given in Table 1 were analyzed. Though most of the experimental work was for methodical reasons done on BEHANIT, the results were verified and found valid also for structural steels in Table 1. Unless stated otherwise, the results presented in the following text will apply to BEHANIT.

An extensive experimental program given in more detail in [11–14] has been carried out in the transition temperature region of materials in Table 1. This program consisted of:

Table 1. Chemical composition of the test material [wt.%]

Steel	C	Mn	Si	P	S	Ni	Al	Ti	Nb	Mo	B
BEHANIT	0.03	0.19	0.13	0.027	0.027						
E 380	0.082	0.92	0.3	0.015	0.014		0.05		0.029		
E 700	0.11	1.81	0.04	0.012	0.01		0.09	0.03	0.06	0.36	0.004
22K	0.21	0.86	0.37	0.021	0.019	0.3				0.12	

1. Mechanical tests:

– tensile tests at strain rates appr. 3×10^{-3} s^{-1}. Flat specimens, cross-section 2×25 mm, the width of deformed area reduced to 5 mm, cross-head speed 0.03 mm/s,

– tensile tests at strain rates appr. 10^2 s^{-1} (electro-hydraulic test machine). Flat specimens as above, cross-head speed 1 m/s,

– standard Charpy impact tests,

– three-point bend static fracture toughness tests.

2. Light and SEM analysis of the deformed area in the vicinity of the main crack. The distribution of slip bands and their interaction with deformation twins were observed on pre-polished surfaces of test specimens. The extent of deformation twinning in the bulk of the experimental material was observed on the etched cross--sections of the specimens.

3. Fractographic analysis of broken specimens.

2.2 Results

The mechanical tests in the transition temperature region [11, 12, 13, 14] shoved a correlation between the deformation mode (twinning) and the fracture mode (cleavage) independently of temperature, strain rate, grain size, testing method, and the type of material. Deformation twinning appeared at slightly higher temperatures and/or lower strain rates than the DBT, thus slightly preceding the occurrence of cleavage. Twins were also observed in regions without visible slip bands, thus they had to form in the very early stages of plastic deformation. In specimens with ductile fracture mode the twins were not found.

SEM analysis of the pre-polished surfaces of test specimens revealed, that most probably depending on the mutual orientation of the twin and the intersecting active slip system, some of the twin boundaries acted as efficient barrier for the slip dislocations, while in other cases slip dislocations could cross the twin boundary. Twin boundary acting as an obstacle for the slip dislocations can be seen in Fig. 1, in which the slip bands diminish in the close vicinity of the twin. Slip bands crossing the twin boundary are given in Fig. 2.

The efficiency of the barrier occurring on some twin boundaries are illustrated in Fig. 3, in which different stages of crack nucleation are visible. Only few separated microvoids appeared on the twin boundary labeled A. Different stages of microcracking at the twin boundary are visible at twins labeled B and C. The frequent occurrence of characteristic zigzag shape of the twin boundary (twin B) seemed to precede the occurrence of typical zigzag shaped microcracks at blocked slip systems.

Fractographic observations supported the assumed significance of the mutual orientation of the twin and the intersecting slip system. Cleavage rivers, observed as slip bands on the pre-polished surface, ran in some cases through the twin

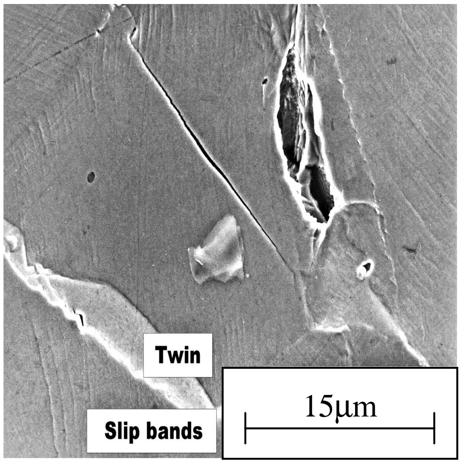

Fig. 1. Twin boundary acting as an obstacle for slip dislocations.

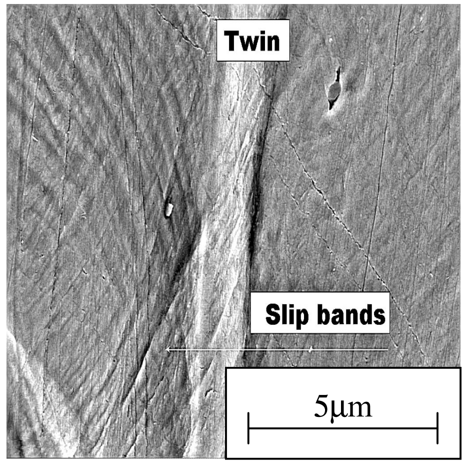

Fig. 2. Slip bands crossing the twin boundary.

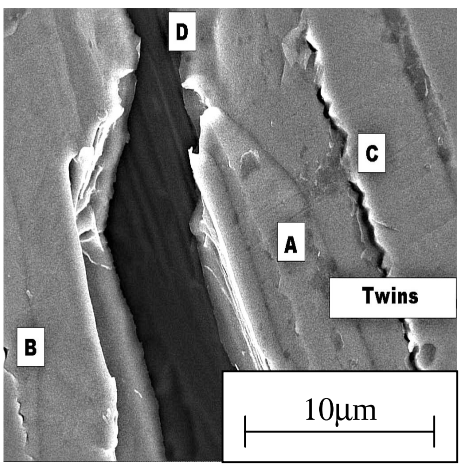

Fig. 3. Different stages of crack nucleation on the twin boundary.

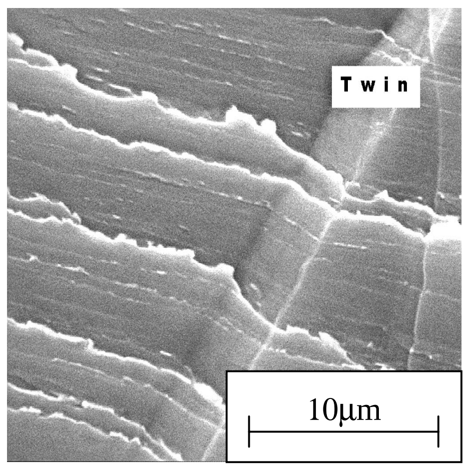

Fig. 4. Cleavage rivers running through the twin boundary.

boundary (Fig. 4), whilst in others they were terminated by the twin boundary (Fig. 5). Fig. 6 illustrates at higher magnification the origin of the zigzag shape of the twin boundary and the associated microcracks. The jagged boundary with

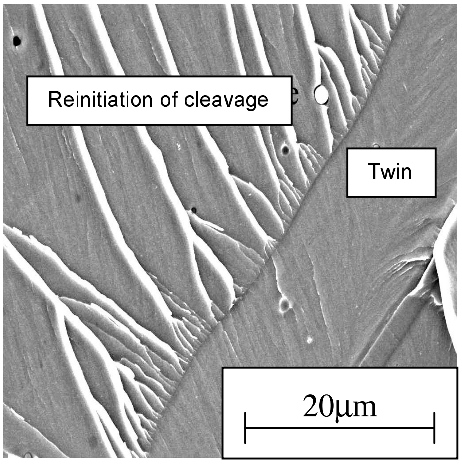

Fig. 5. Cleavage rivers terminated by the twin boundary.

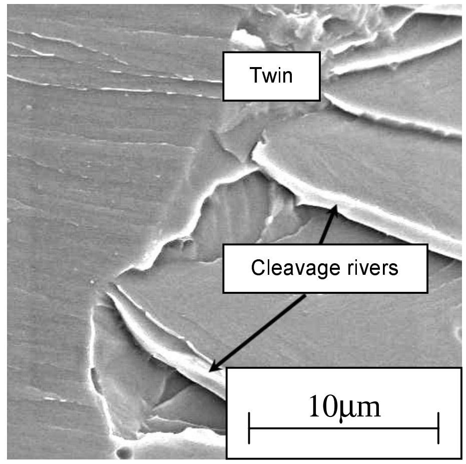

Fig. 6. The origin of the zigzag shape of the twin boundary and the associated microcrack.

microcracks, observed on the pre-polished surfaces of test specimens, is obviously a consequence of the interaction of active slip systems with unfavorably oriented twin boundary, blocking the further movement of slip dislocations.

Detailed analysis of the polished cross-sections of tested specimens revealed numerous microcracks in the vicinity of the cleavage main crack in all specimens. The occurrence of microcracks was restricted to distances up to several grain diameters from the main crack. Since similar defects could not initiate in the "stress shadow" below or above the growing main crack, it has to be admitted, that they initiated in the stress/strain field of the approaching main crack tip. These microcracks will be further referred to as *pre-cleavage microcracks (PCMC)*.

Etching revealed a strong tendency to deformation twinning in the areas with the occurrence of PCMCs. Both features are demonstrated in Fig. 7. In the case of mixed ductile/cleavage fracture mode, the occurrence of both PCMCs and twins was strictly restricted to the neighborhood of cleavage facets.

Furthermore, the association of PCMCs with deformation twins was manifested on the etched cross-sections of tested specimens. As shown in Fig. 8, PCMCs exhibited concordant orientation with the deformation twin boundaries. The relatively opened PCMC in Fig. 9 obviously follows the twin boundary. The characteristic wedge-shaped nature of cavities on the boundary of deformation twins, which represents the nuclei of the cleavage facet, is visible in Fig. 10.

Fig. 11 demonstrates the complex nature of the failure in the vicinity of the main crack and the significance of deformation twins for cleavage fracture initia-

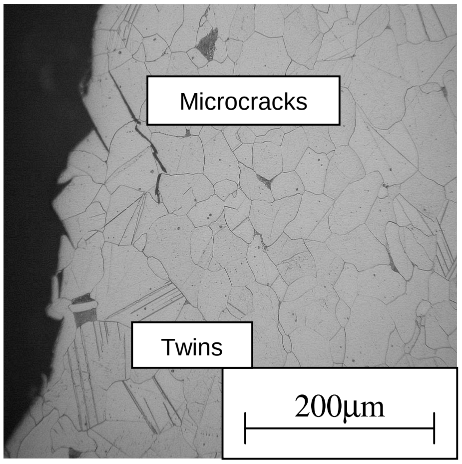

Fig. 7. Strong tendency to deformation twinning in the area of PCMCs.

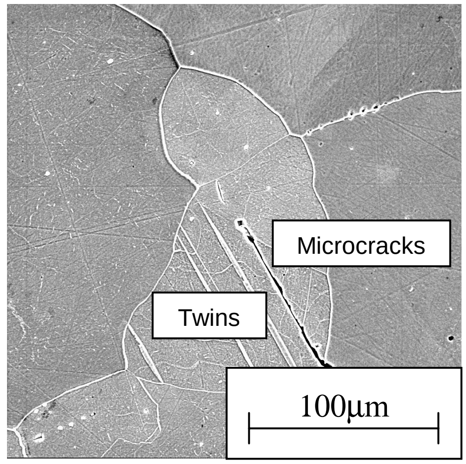

Fig. 8. Association of PCMCs with deformation twinning.

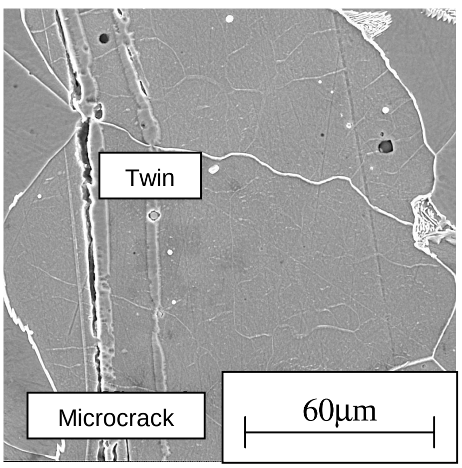

Fig. 9. PCMC along the twin boundary.

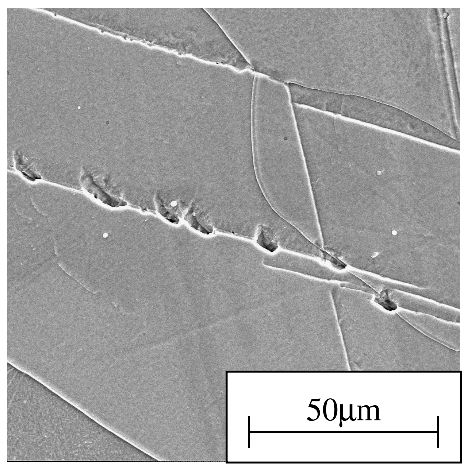

Fig. 10. Characteristic wedge-shaped nature of cavities on the boundary of deformation twins.

tion. Both cracked twin boundary and the nucleation of cavities on both sides of high angle grain boundary and the irregularly cracked eutectoid grain can be seen. Comparing Fig. 10 and Fig. 11, the difference between the defects nucleated on the

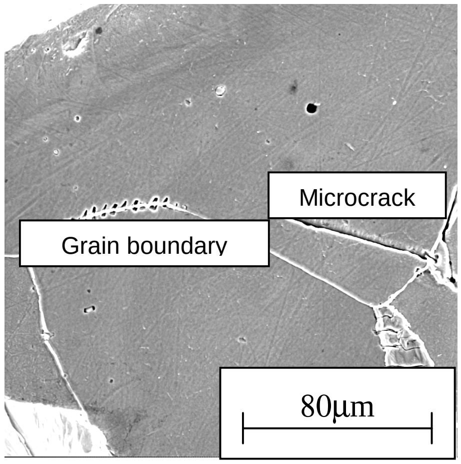

Fig. 11. Complex nature of the failure in the vicinity of the main crack.

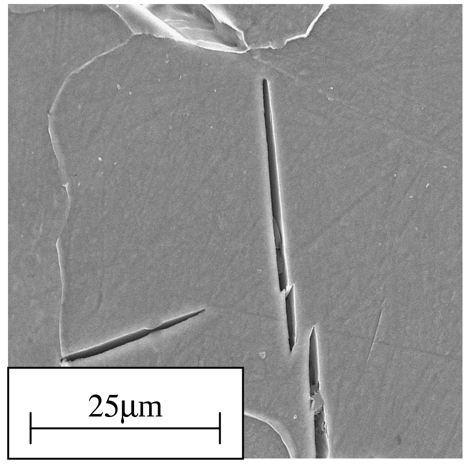

Fig. 12. "Jumps" of the fracture plane of the PCMC into the adjacent parallel plane.

twin boundary and on the large angle grain boundary can be observed: cleavage facets are initiated on the twin boundary[1] whereas the dimples of ductile fracture develop on the grain boundary.

One of the frequently observed features of PCMCs in all types of analyzed materials were "jumps" of the fracture plane of the PCMC into the adjacent parallel plane. An example observed in K22 steel is given in Fig. 12. The reason of these jumps is demonstrated in Fig. 13, in which an agglomeration of inter-linked parallel deformation twins in the same area is shown. The jumps of the PCMC's cleavage plane on the set of inter-linked parallel twins were observed on the fracture surface as sets of parallel steps. An example of such steps in K22 is shown in Fig. 14. The fracture mode between the cleavage facets of PCMCs, i.e. between the re-initiation sites of cleavage fracture, varied from the ductile to brittle one. Ductile bridges interconnect the cleavage facets in Fig. 14.

Fractographic analysis did not reveal carbide (or other brittle) secondary particles in the cleavage (re)initiation sites. Moreover, secondary particles, found in the active slip system, proved to be harmless (Fig. 5). The morphology and distribution of slip bands on cleavage facets (cleavage rivers) confirmed the frequent re-initiation of cleavage on the twin boundary (Fig. 5).

The re-initiation of cleavage fracture on the twin boundary was proved at temperature as high as +20 ℃. Furthermore the shape of cleavage rivers frequently indicated the re-initiation of cleavage ahead of the ductile crack growth region, as

[1] intersecting slip bands cannot be observed on the polished cross-section

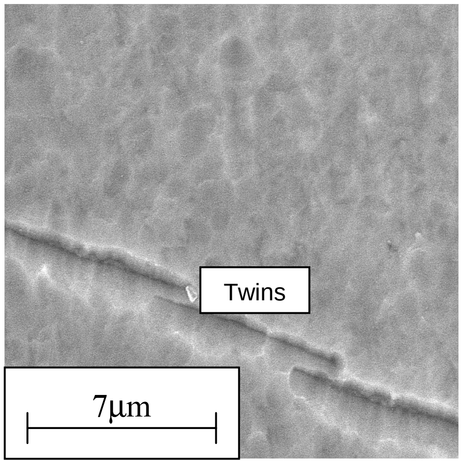

Fig. 13. The reason of the jumps in Fig. 12.

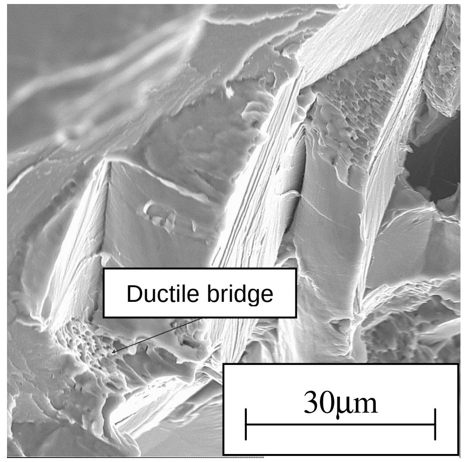

Fig. 14. Jumps of the fracture plane of the PCMC as observed on the fracture surface.

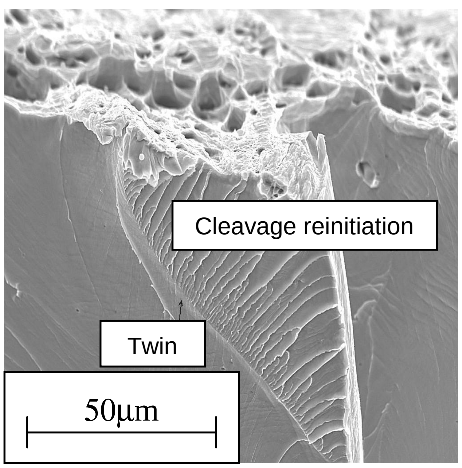

Fig. 15. Initiation of cleavage ahead of the ductile crack growth region.

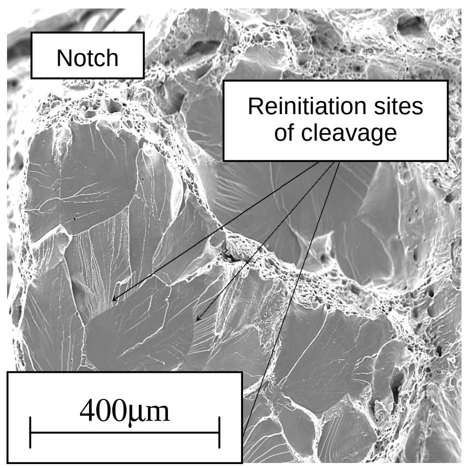

Fig. 16. As Fig. 15, lower magnification.

documented in Fig. 15 at higher magnification and in Fig. 16 at lower magnification. Fig. 16 shows a relatively low magnification SEM micrograph of the fracture surface after the Charpy V-notch impact test at +20 °C. The depicted region neighbors the notch (upper left part of the Fig. 16) and the surface of the specimen (upper right part of the Fig. 16). The narrow regions of ductile fracture below the notch and the specimen surface delimit the volume of the specimen in which the plastic deformation, finally leading to rupture of the specimen, started. Though the overall direction of the main crack growth was *to* the bulk of the specimen, i.e. *away from the ductile regions*, locally, as indicated by cleavage rivers patterns, the cleavage facets grew *towards the ductile regions*.

2.3 Discussion

The most important experimental results can be summarized as follows:

– Correlation between the deformation mode (twinning) and the fracture mode (cleavage) under various deformation conditions was found in tested materials.

– Deformation twinning occurred in the very early stages of plastic deformation and at temperatures (strain rates) slightly higher (lower) then the observed DBT and cleavage fracture.

– No cracked brittle particles were observed in the initiation and re-initiation sites of cleavage.

– Cleavage fracture (re)initiation was proved at the intersections of active slip systems with unfavorably oriented deformation twins.

– Frequent brittle microcracks (PCMC), which might only initiate ahead of the approaching main crack tip, were observed in the vicinity of main cleavage crack.

– PCMCs were associated with deformation twins.

– Initiation of the cleavage crack on deformation twin ahead of the ductile fracture region was proved.

The above mentioned results logically cast doubts on the independence of DBT and deformation twinning, i.e. whether twinning and DBT really are two independent processes, which happen to occur in the same temperature and strain rate range, as suggested by Reid [8]. Our scanning electron microscopic observations rather indicate that deformation twinning seems to be an important and integral part of plastic deformation in the stress-strain field of the moving main crack tip in the transition and sub-transition temperature region. Moreover, the mechanism of cleavage crack initiation on the intersections of active slip systems with deformation twins, originally proposed by Biggs and Pratt [15] for cryogenic temperatures, is most probably able to generate cleavage crack nuclei (PCMCs) also ahead of the moving main crack tip and at temperatures up to the DBT temperature.

The suggestion of deformation twinning providing the nucleation sites for PCMCs ahead of the rapidly moving cleavage crack tip in bcc ferritic steels is not in any contradiction with the literature data. Unlike the fcc metals, deformation twinning in bcc metals (ferritic steels) really occurs in the very early stages of plastic deformation, often before an obvious slip of dislocations [9]. The transsonic rate of twin growth was proposed experimentally [16] and by atomistic simulations as well [17, 18, 19]. The results in [19, 20] suggest, that the twin growth rate exceeds the rate of brittle crack growth. Thus, deformation twinning fulfils the fundamental requirements for its possible participation in the brittle fracture: generation of deformation twins before an extensive slip and this ahead of the rapidly growing main crack tip.

Since from the crystallographic point of view the transition of matrix slip dislocations through the twin boundary is in general always possible [21], the nucleation of wedge-type microcracks on the intersections of active slip systems with deformation twins in ferritic steels will be most probably associated with the existence of a mid-rib with a high density of dislocations in the central part of deformation twins in bcc metals. The very thin mid-rib [10], representing a nucleus of deformation twin in bcc metals, is supposed to form dynamically at the onset of twinning and increases its thickness under the external stress most probably by one of the suggested pole mechanisms for twin growth. The high density of dislocations in the mid-rib is likely to contribute to the energetic barrier for matrix dislocations, which according to kinematic calculations, exists on the twin boundary [22, 23].

Due to its planar character, the twin boundary can intersect many active slip systems (as demonstrated in Fig. 5) and large elastic strain energy of the lattice can thus be accumulated in the vicinity of the unfavorably oriented twin. The elastic strain energy stored in the vicinity of the twin thus significantly exceeds the energy accumulated at other possible obstacles for dislocation motion (e.g. hard secondary particle in Fig. 5). The large elastic strain energy accumulated in the vicinity of the twin favors the fast initial growth of the crack nuclei.

The observed direction of the propagation of cleavage, re-initiated on the twin boundary, can be considered to be another important result. As indicated by the shape of cleavage rivers in the marginal regions of the specimens, PCMCs grew towards the main crack tip. This observation is again in full agreement with the assumed nucleation of cleavage microcrack ahead of the notch or pre-crack and the non-continuity of the cleavage main crack growth [3].

3. Proposed mechanism of DBT and cleavage fracture of ferritic steel

Based on the experimental results and the literature survey a mechanism of non-continuous cleavage main crack initiation and extension by nucleation and growth of "inherent" microcracks (PCMCs) on the deformation twins, generated ahead of the moving main crack tip, can be proposed. The model is based on the micromechanism of cleavage crack initiation suggested by Biggs and Pratt for single crystals at cryogenic temperatures [15]. However, we suppose that similar mechanism (schematically presented in Fig. 17) operates repeatedly in the stress field of the moving main crack tip and even in the transition temperature region. The twins nucleate in the early stage of deformation in the plastically strained volume around the stress raiser (e.g. notch) or main crack tip. In the course of further plastic strain dislocations pile up on the intersections of active slip systems with unfavorably oriented twins. PCMCs, initiated on the twins ahead the main crack tip, extend towards the developing crack. According to the number of dislocations piled up at the twin boundary, cavities (the boundary of the twin labeled "A" in Fig. 3), microcracks with a typical zigzag shape (the twin labeled "B" in Fig. 3) or PCMCs (the twin labeled "C" in Fig. 3) can be formed along the twin boundary.

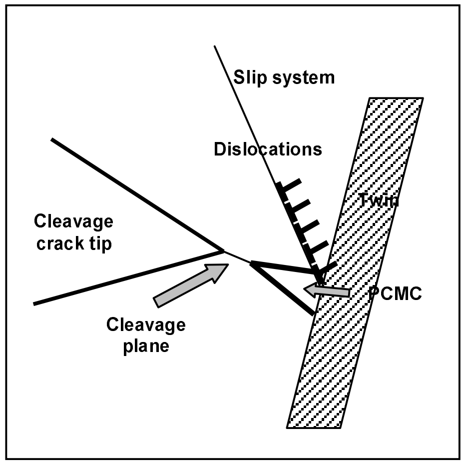

Fig. 17. Schematic representation of cleavage fracture.

Depending on the loading conditions and the properties of the material affecting the extent of twinning (i.e. their spacing) the failure of the bridges between the first PCMCs in the course of further loading can be ductile or brittle. The brittle-ductile behavior may further depend also on the orientation of microcracks and on the tensile and shear strength in the individual surrounding (proper) crystalline directions.

Once the first few PCMCs are connected and the nucleus of the main crack is formed, the process of twin generation ahead of the growing main crack nucleus tip is accelerated due to the higher crack tip concentration effect. The growth of the cleavage crack appears in the form of jumps of the nearest favorably oriented PCMC to the main crack tip. Due to the intrinsic tendency of the ferritic material to blunt the crack tip, the cleavage mode of crack propagation will be directly related to and controlled by the process of twin generation and nucleation of PCMCs ahead of the growing crack tip. An entirely cleavage mode of fracture will appear providing the spacing of PCMCs on twins ahead of the growing crack tip is sufficiently small.

Thus, the cleavage fracture of bcc materials in the above model represents the result of combined processes of deformation twinning and slip of matrix dislocations in the stress-strain field of the moving main crack tip. The model provides an explanation of the origin of the predicted inherent cleavage crack nuclei in ferritic matrix as well as of the assumed non-continuity of the cleavage crack propagation in the material with intrinsic tendency to blunt the sharp crack tip. Both follow directly from the proposed generation of twins and PCMCs at stress raisers during initial loading and later ahead of the growing crack tip.

4. The principal controlling parameters of DBT and cleavage fracture in ferritic steels

The model of DBT and cleavage based on the combined effect of deformation twinning and slip of dislocations in front of the propagating crack tip is in good correlation with the experimentally found influence of the main material parameters, controlling both DBT and deformation twinning in ferritic steels.

The principal parameters affecting the DBT of the steel are grain size and microstructure, while deformation twinning is known to be favored by large grain size, lack of mobile dislocations and solid solution hardening (e.g. [10]). Obviously, the frequently demonstrated prime influence of the grain size on the DBT temperature (e.g. in [25]) is in good agreement with the proposed model. Since the size of PCMCs is limited by the size of the twins, i.e. the grain size, the increased grain size means simultaneously more and larger twins as well as PCMCs nucleated on them in front of the crack tip. Closer spaced and larger PCMCs promote cleavage fracture and thus increase the DBT temperature. Thus, grain refinement increases the strength and simultaneously decreases the DBT.

The basic strengthening mechanisms (besides the above mentioned grain refinement) used to achieve the required mechanical properties in the steel metallurgy are strongly inter-related with the resulting microstructure of ferritic steels: precipitation hardening, solute solution hardening and transformation hardening (i.e. the density and configuration of dislocations). Secondary hardening is known to increase the DBT temperature, and through its strengthening effect it should promote also twinning. Solute solution strengthening promotes deformation twinning and hence should increase the DBT. The density and configuration of dislocations can affect the tendency to deformation twinning, and thus, the DBT as well through the available population of mobile dislocations and/or through the effect of existing density of dislocations upon the process of blunting the sharp crack tip (emission or absorption of dislocations).

Thus, various strengthening mechanisms may affect the tendency to deformation twinning and the DBT in different ways. Since their relative contribution to the strength of the steel can vary from case to case, any simple relation between the mechanical properties, microstructure and the DBT is unlikely. However, keeping the basic microstructural parameters (grain size and type of microstructure) constant, any increase of the strength of the matrix should increase the probability of DBT, since it increases the probability of achieving the stress required for deformation twinning(2) in the course of further plastic strain.

(2) usually higher than yield stress

5. Conclusion

Based on the recent experimental results published in detail elsewhere [11–14], it was proposed that deformation twinning represents an integral part of deformation processes in the propagating crack tip region of cleavage fracture. A new model of cleavage fracture and DBT was proposed, in which deformation twins developing in front of the moving main crack tip can act as nucleation sites for cleavage fracture nuclei. Their size corresponds to that of the inherent nuclei of cleavage cracks, predicted by the theory of brittle/cleavage fracture which, however, have not hitherto been observed in ferritic materials. The assumed initiation and reinitiation of cleavage fracture on deformation twins in front of the propagating cleavage crack tip might probably eliminate the discrepancy between experimental results and the theory of brittle/cleavage fracture.

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