



FATIGUE CRACK INITIATION IN FCC SINGLE CRYSTALS

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ABSTRACT

Initiation of fatigue cracks both in model fcc single crystals and in fcc single crystals used in engineering practice is discussed. The emphasis is placed on the role of different types of cyclic slip localisation. It is shown that the phenomenon of persistent slip bands (PSBs) is confined to single crystals of sufficiently high stacking fault energy cycled at a relatively narrow range of loading conditions. For single crystals of not suitable orientations and/or of low stacking fault energy cycled under stresses and/or strains outside the critical range and/or under high temperatures the cyclic plasticity manifests itself by other forms of slip activity leading to the formation of surface hill-valley topography. The necessary prerequisites for the microcrack initiation are (i) expressive notch-peak topography, (ii) locally higher cyclic plastic strain at the intrusion root, and (iii) presence of suitable dislocation configuration around the surface intrusions. The existing models of crack initiation are accessed in the light of these prerequisites.

KEYWORDS

Cyclic plastic deformation, crystal defects, fatigue crack initiation, dislocation structures.

INTRODUCTION

Experimental observations have shown that in homogeneous flaw-free materials, microcracks mostly often originate at free surfaces. This is valid generally for polycrystalline and monocrystalline materials. For example, it has been repeatedly demonstrated that when a specimen is fatigued for a substantial fraction of its fatigue life and its surface is then removed by electropolishing, the specimen in a subsequent test exhibits a fatigue life as long as that of a virgin specimen. Single crystals are used not only for basic studies of mechanisms of plastic deformation, but also in the engineering structures. The best known case is represented by superalloy single crystals used for the production of critical parts of gas turbines. In these single crystals the cracks initiate at pores lying at or near surface. Crack initiation, as well as the whole fatigue process, is controlled by the cyclic plastic deformation. Thus these initiation sites are also sites of higher cyclic slip activity. The mechanisms of the initiation are still a matter of speculation. There is also no generally accepted quantitative description of the initiation process and consequently it is not possible to perform numerical analysis of the initiation. The aim of the present paper is to discuss the general prerequisites of the crack initiation in fcc single crystals and to assess the mechanisms proposed for the initiation process.

FORMATION OF SURFACE RELIEF

Single crystals of pure metals

The most prominent feature of cyclic plasticity is formation of persistent slip bands (PSBs) in some metals under suitable conditions. The role of PSBs in fatigue was overestimated in the past. Therefore their properties, structure and especially the requirements for their formation will be one of the central themes of this section. The PSBs have been most extensively studied on copper single crystals. Fig. 1 shows structure of PSB a few microns below surface of copper single crystal cycled at a low stress amplitude. The structure of the PSB, lying along

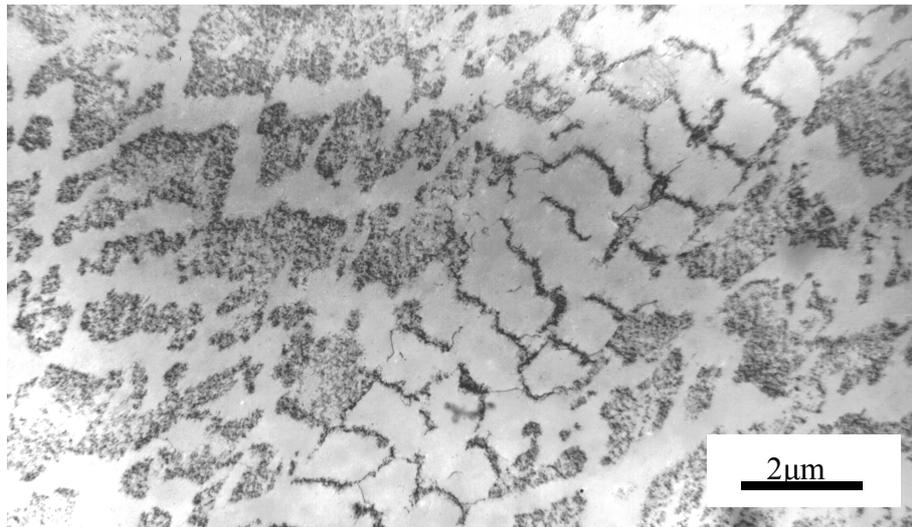


Fig. 1. Persistent slip band in cycled single-slip-oriented copper single crystal. TEM, section perpendicular to primary slip plane.

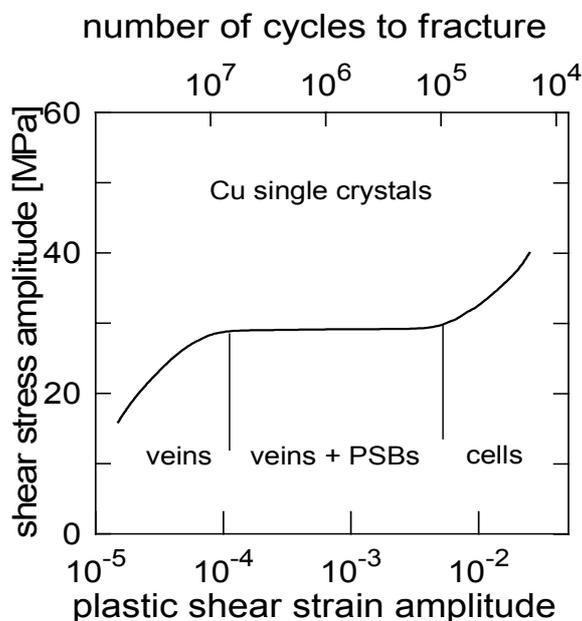


Fig. 2. Cyclic stress-strain curve of single-slip-oriented copper single crystals obtained at symmetrical plastic-strain-controlled cycling. Corresponding fatigue lives and the regions of different dislocation structures are also indicated.

the primary slip plane, resembles here three irregular ladders, while the surrounding matrix structure is one of perpendicularly cut veins. The cyclic plastic strain amplitude in PSBs is higher than in the surrounding matrix; in copper single crystal it is higher by a factor of about 100. There are certain stress and strain requirements for PSBs formation. PSBs have never been observed below a threshold value of the plastic strain amplitude. This threshold is typically of the order of 10^{-5} . They have not been observed at high strain amplitudes at symmetrical cycling. Fig. 2 shows the cyclic stress-strain curve (CSSC) of copper single

crystals oriented for single slip [1] together with fatigue life data obtained in strain-controlled tests by Cheng and Laird [2]. Dislocation structure produced by cycling with the shear plastic strain amplitude $7 \times 10^{-5} < \gamma_{ap} < 7 \times 10^{-3}$ consists of veins and PSBs (Fig. 1); the volume fraction of the PSBs increases with increasing strain amplitude over the plateau in the CSSC from zero to 100 %. It can be seen that the co-ordinates of the PSB threshold are $\tau_a = 28$ MPa and $\gamma_{ap} = 7 \times 10^{-5}$. The CSSC and fatigue life data presented in Fig. 2 are valid only for symmetrical plastic strain controlled cycling. Later investigations show that the cyclic stress-strain response of copper single crystals very strongly depends on the regime of cycling, or in other words on the loading history. For example, Melisova et al. [3] cycled copper single crystals under stress control with the desired stress amplitude reached in the first half-cycle. No plateau in the CSSC was found, but PSBs in the structure were found with the threshold given by $\tau_a = 19$ MPa and $\gamma_{ap} = 7 \times 10^{-5}$.

The PSBs cannot be detected on the specimen surface right from the onset of cycling, but rather only at the end of hardening process when the interior structure is already formed. Therefore, PSBs are probably formed by transferring the matrix structure into the PSB structure. During the early stages of cycling, the interior structure is formed, and simultaneously fine slip lines appear on the specimen surface because dislocations are escaping to the free surface. At or near the surface, the stress in localised places can exceed average. Because of the instability of the interior structure, the dislocation structure in such places must respond to the increased stress and form the PSB. The cyclic plastic strain within these PSBs leads to formation of surface intrusions and extrusions, which in turn give rise to stress concentration and thus enhance the process of PSBs broadening and growing to greater depths.

Lukáš et al. [4] found that stress-controlled cycling with a non-zero mean stress leads to a substantially different stress-strain response and to a substantially different dislocation structures in comparison to symmetrical cycling. Namely, it was found that there is no plateau in the CSSC and that the dislocation structure is a homogeneous cell structure with the cells arranged in slabs lying predominantly along the primary slip plane. This indicates that the PSBs in single-slip-oriented copper single crystals are only formed at symmetrical or nearly symmetrical cycling. Stress-controlled experiments performed on polycrystalline wavy-slip

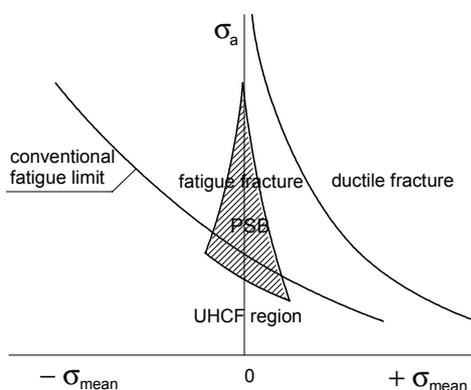


Fig. 3. Stress requirements for formation of PSBs in wavy-slip fcc metals.

sliding of the layers of cells for the stress and/or strain amplitudes above the conventional

fcc metals copper [5] and nickel [6] show the same. The experimental data are sufficient to tentatively construct a schematic diagram showing stress requirements for the formation of the PSBs in wavy-slip fcc metals at temperatures not exceeding about 400 °C; for higher temperatures no PSBs were found in the structure [7]. This diagram is shown in Fig. 3. The dislocation structure in the hatched area consists of two phases (ladder-like or cell-like zones embedded in vein structure), the structure outside the hatched area consists of one phase, namely of veins below the hatched area and of cells everywhere else. Within the hatched area the surface slip bands are clearly related to the PSBs. Outside the hatched area there are also intensive surface slip bands. They are due to the relative

fatigue limit. This sliding also produces surface intrusions and thus represents the main preparatory step for the crack initiation.

The cyclic stress-strain response of copper single crystals is insensitive to the frequency of cycling. Buchinger et al. [8] found the PSB threshold and the plateau stress to be $\tau_a = 26$ MPa in copper crystals cycled at 20 kHz. On the other hand, cycling of polycrystalline copper at ultrasonic frequencies [e.g.9] proved that the failure can occur at 10^{10} cycles at stresses well below the conventional fatigue limit, i.e. below the PSB-threshold. In this gigacycle region PSBs do not form and the mechanism of failure is related to the cyclic slip irreversibility. This small irreversibility repeated $10^8 - 10^{10}$ times can also lead to the formation of sufficiently intensive surface valley and hill topography and thus prepare the soil for the microcrack initiation [10].

Single crystals of alloys

Alloying of fcc single crystals generally decreases stacking fault energy and consequently changes the slip mode from wavy slip to planar slip for high enough content of the alloying element. In planar-slip metals (like Cu-Al and Cu-Zn alloys with electron-atom ratio higher

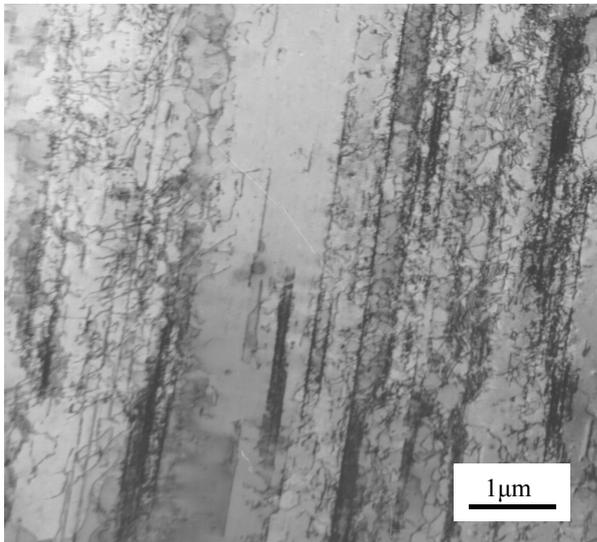


Fig. 4. Planar array arrangement in cycled single-slip-oriented single crystal Cu-22%Zn. TEM, section perpendicular to primary slip plane.

then 1.19 [11]) a more or less regular hill and valley surface morphology was found many times after sufficiently high number of loading cycles; the surface relief is not related to any specific dislocation structure. Here the surface relief results from the irreversible random (at low amplitudes) or quasi-random (at higher amplitudes) cyclic slip. The dislocation structure produced by cycling with lower plastic strain amplitudes consists of planar arrays of edge dislocations on the slip planes. Example of this structure is shown in Fig. 4. It can be seen that there are denser and less dense slabs; this witnesses a certain inhomogeneity of the cyclic slip. Such slabs of activated primary slip planes are often called "persistent Lüder's bands" (PLBs) [12]. These bands are assumed to represent zones of localised cyclic slip. Contrary to the PSBs, PLBs are not permanent and do

not represent zones of dislocation structure different from surrounding matrix. The PLBs are not stable – the localised strain moves around the gauge length and the active life of the slip bands is short. The shown type of structure is typical for all the difficult-cross-slip crystals.

Engineering single crystals

Superalloy single crystals are used for the production of blades and vanes of gas turbines. The microstructure of these alloys consists of a γ matrix in which cuboidal γ' precipitates are coherently embedded. The volume fraction of γ' precipitates is typically about 60 to 70 %, the size of γ' cubes (measured along the cube edge) is about $0.5 \mu\text{m}$ and γ/γ' interfaces are aligned to $\{001\}$ planes. Fig. 5 shows this structure. Initiation of fatigue microcracks occurs at

micropores and in some alloys also at carbides (when enough carbon is present in the alloy). The γ' precipitates represent the harder phase. The deformation takes place predominantly by generation and glide of dislocations of the type $\{111\}\langle 110\rangle$ in γ channels. At higher amplitudes the dislocations generated in the γ channels can cut through the γ' precipitates. Cyclic slip localisation in the form of PSBs has been observed at relatively low temperatures

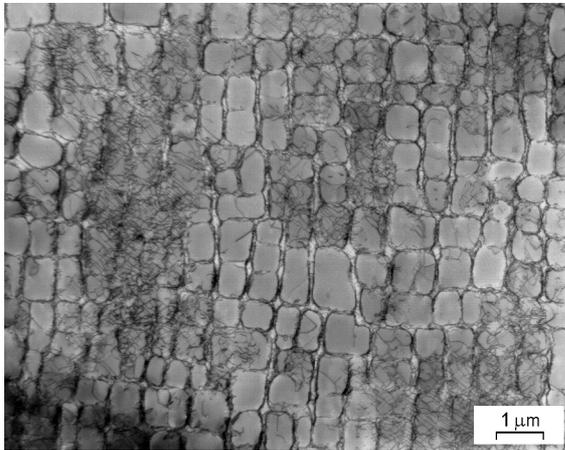


Fig. 5. γ/γ' structure of superalloy single crystal CMSX-4.

below 760 °C [13-17]. At higher temperatures (above 760 °C) no PSBs were found. One example of the PSB structure is shown in Fig. 6 [17]. This TEM micrograph shows the structure of $\langle 001\rangle$ -oriented single crystal CMSX-4 cycled at 700 °C; the section contains the stress axis and is perpendicular to the slip plane (111) along which the PSBs run across the whole crystal. The PSBs appear here as very thin slabs (thickness below 0.1 μm) going through both the γ channels and the γ' particles. The dislocation within the PSBs cannot be resolved. Fig. 7 [17] shows the PSBs observed by using scanning electron microscopy of the surface of cycled specimen. The PSBs can be seen here as white bands along the

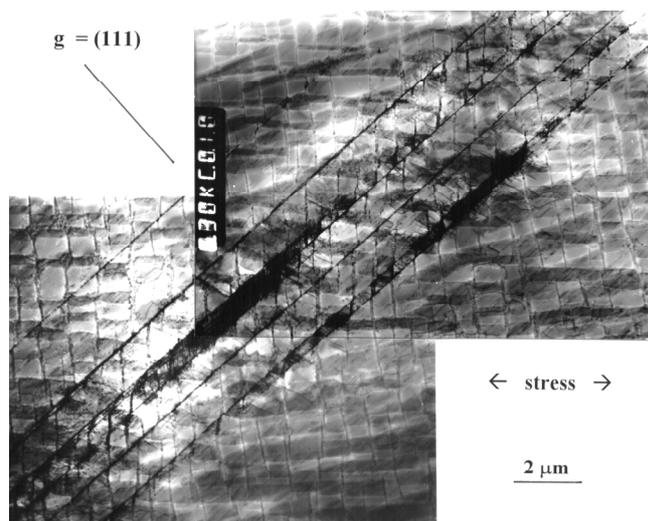


Fig. 6. Persistent slip bands in $\langle 001\rangle$ -oriented superalloy single crystal CMSX-4 cycled at 700°C. TEM, section perpendicular to slip plane (111).

the (111) plane. The much shorter and less regular lines along the trace of the (001) plane correspond to the horizontal γ channels perpendicular to the stress axis. These lines are probably formed by the slip activity of more slip systems of the type $\{111\}\langle 001\rangle$ operating in the γ channels. Their activity results in "squeezing out" or "sucking in" of the γ matrix in between the harder γ' particles. It should be stressed that the PSBs shown in Figs. 6 and 7 could be seen only at specimens cycled at higher total strain amplitudes at 700 °C. At low amplitudes at 700 °C the PSBs were not observed. The same holds for arbitrary amplitude at 850 °C and 950 °C. Thus it can be concluded that the surface relief at lower temperatures is formed both by PSBs and activity of the horizontal γ channels. At higher temperatures only the horizontal γ channel form the surface slip markings.

This section can be concluded by the statement that the cyclic plastic deformation results in all the cases in the formation of the surface relief. The surface relief is in some cases connected with a clear slip localisation and specific dislocation structures, in other cases there is no such a connection.

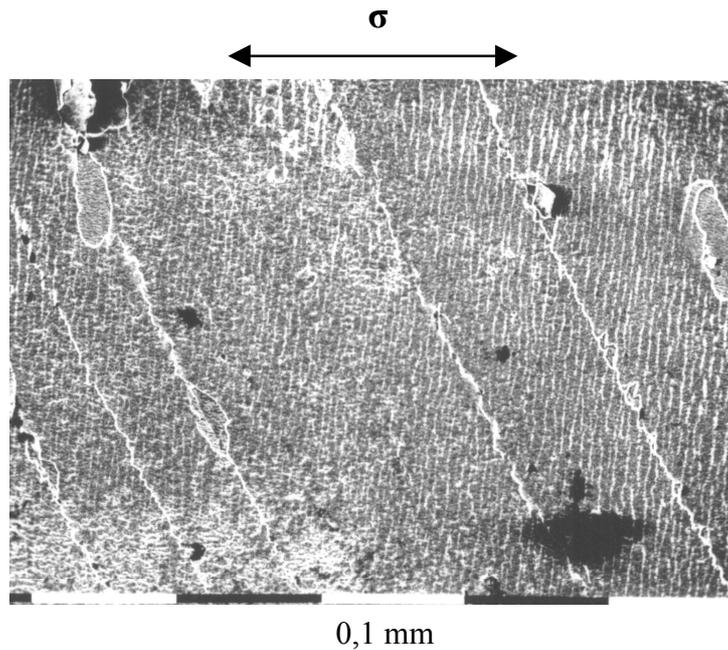


Fig.7. Surface relief of $\langle 001 \rangle$ -oriented superalloy single crystal CMSX-4 cycled at 700°C . SEM, section perpendicular to slip plane (111).

GENERAL CONDITIONS FOR CRACK INITIATION

It was already stressed that the cracks initiate either at specimen surface or at pores lying at or near surface. In the case of superalloy crystals the micropores serve as stress concentrators, their inner surface represents the free surface at which the process of initiation takes place. The initiation can be treated along the same lines as in model materials; the stress concentration locally enhances the dislocation processes. Surface intrusions formed by the cyclic plastic deformation (together with surface extrusions) are the exact sites of the initiation. In easy-cross-slip crystals the surface slip relief is related to the slip activity of the PSBs for suitable region of loading parameters (Fig. 3) and for not too high temperatures. For other cases above the conventional fatigue limit it is the repeated and only partly reversible sliding of the whole slabs of cells along the slip planes which leads to the gradual formation of the surface slip markings. In the gigacycle regime it is the local cyclic slip irreversibility which very slowly builds up the surface relief. In difficult-cross-slip crystals, the irreversible part of the motion of dislocations in planar arrays leads to the planar hill and valley surface topography. In superalloy crystals, activity of PSBs and/or horizontal γ channels forms the necessary surface relief not only on the flat outer surfaces, but also on the inner surfaces of pores; in the latter case it can be expected that the intensity of formation is enhanced by the stress raising effect.

The crack initiation is an irreversible process, which is preceded by irreversible dislocation processes in the critical volumes. The necessary prerequisites for the microcrack initiation are (i) expressive notch-peak topography, (ii) locally higher cyclic plastic strain at the intrusion root, and (iii) presence of suitable dislocation configuration around the surface intrusions. The notch-peak topography causes geometrical stress concentration. This would not suffice; the intensity of the irreversible cyclic plastic deformation, i.e. the irreversible part of the

dislocation glide, has to be higher at the intrusion root than in other places. This requires such dislocation structure which prevents local stress relaxation by unimpeded glide of dislocations out of the critical volume and simultaneously contributes to the intrusion root sharpening and not to its blunting. For these purposes the presence of suitable dislocation configuration is needed. The three conditions are interconnected and are not conceivable separately. For example, a sharp artificial scratch on the surface of copper single crystal need not become the site of crack initiation in subsequent cycling, in spite of the fact that it represents a stress raiser. The reason is that the proper local dislocation configuration guaranteeing the fulfilment of the last two conditions is missing.

MODELS OF CRACK INITIATION

For initiation of microcracks, a large number of models have been proposed. The proposed mechanisms applicable to single crystals can be roughly divided into four groups:

1. *Models which do not distinguish between intrusion and microcrack.* In this case, microcrack formation is identical with continuous growth of intrusion into the depth of the crystal.

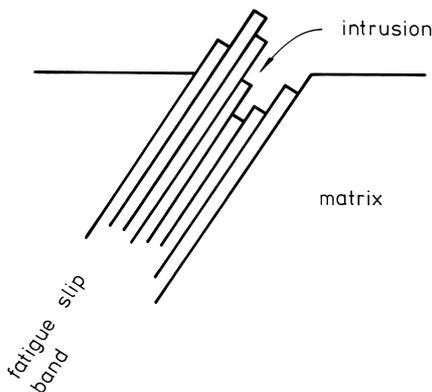


Fig. 8. Model of card slip in fatigue slip band.

This may happen by repeated slip on one or more slip systems. The basic idea for the one-slip-system case is the relative motion of parallel cards (Fig. 8). Wood [18] assumes that the formed intrusion acts as a stress raiser, and promotes further slip just in the "notch root". May [19] showed theoretically on the basis of statistical formalism that with continued cycling, progressively deeper intrusions would result from random slip. Lin et al [20] calculated the relative motion of two non-neighbouring cards or slices. The calculation performed under acceptable assumptions showed that the local plastic shear strain in both slices (one positive and the other negative) can reach very high values within a

relatively short number of cycles. These large plastic strains cause the continuous "squeezing out" or "sucking in" of the layer between the slices. In other words, in the second case we get a continuously deepening intrusion. The model by Lynch [21], also using the idea of soft layers being extruded or intruded during cycling, yields a similar result: the fatigue cracks initiate and grow by a mechanism of intrusion which occurs when soft layers are "sucked in". This mechanism can operate both with and without PSBs. Fig 8 corresponds to the slip localised in the PSB. There are also modern versions of the models of the discussed type represented by the computer simulations of random irreversible slip [22]. Such a model can be well applied e.g. to the initiation in the gigacycle region (see Fig. 3). Neumann [23] proposed a model for the formation of cracks by coarse slip on alternating parallel slip planes (Fig. 9). In this model the crack develops from coarse slip steps: in tension (a) slip plane 1 is activated; excess dislocations of one sign remain on this slip plane. The slip step produced acts as a stress raiser, which also helps to activate slip plane 2 under the same tensile load. This leads to configuration (b) and to excess dislocations of one sign on plane 2. During the text compression, excess dislocations on 1 and 2 run back, thus leading to configuration (c). It is assumed that the surface at A are not "rewelded", i.e. they only touch macroscopically.

Configuration (c) thus already represents a crack nucleus in A. Repetition of this process takes place on further glide planes of the same slip systems, which leads to continuous increase of microcrack length.

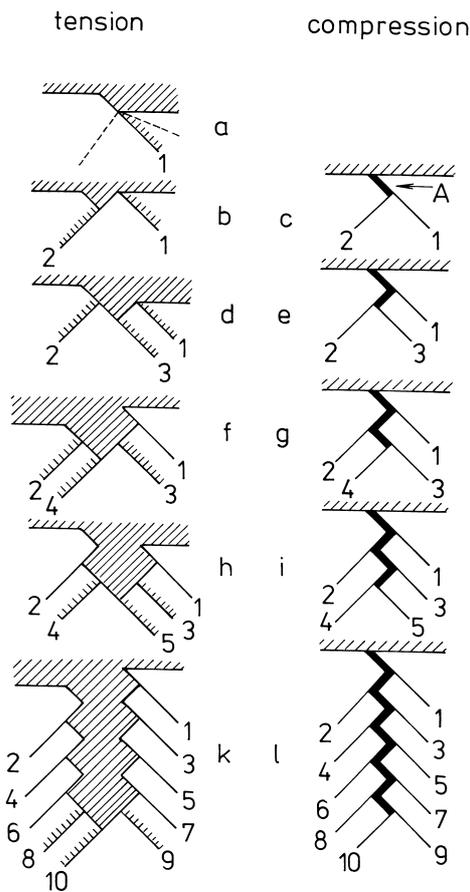


Fig. 9. Neumann's model of crack initiation.

increase in stress or energy, sufficient to destroy crystal coherency in small regions (of the order of nanometers and less) [25,26]. For example, Fujita [25] showed theoretically that the dislocation dipole with small separation of the two components of the dipole can lead via annihilation to crack nucleation.

Summing up, all the mechanisms reviewed have their merits and their justification in experimental findings. None of them has been worked out quantitatively, which would make it possible to express the influence of both the external and internal parameters on the rate of nucleation.

CONCLUSIONS

- Microcracks in fcc single crystals initiate at the sites of higher cyclic slip activity, i.e. either in the surface intrusions or/and at the subsurface pores when present and large enough.
- The necessary prerequisites for the initiation are (i) expressive notch-peak topography, (ii) locally higher cyclic plastic strain at the intrusion root, and (iii) presence of suitable dislocation configuration around the surface intrusions or pore root.
- None of the proposed mechanisms of initiation covers all the experimental findings and none of them has been worked out quantitatively.

2. *Local brittle fracture.* This concept distinguishes clearly between intrusions and cracks. A trivial example of this mechanism is the cracking of a brittle second-phase particle at the site of a stress concentration due to fatigue notch-peak topography. Such a crack can then be overtaken by the basic material. There is a certain probability that this mechanism can also operate at the intrusion root in single-phase materials.

3. *Condensation of vacancies.* Cyclic deformation produces a higher number of vacancies than monotonic loading [24]. This may be due mainly to to-and-fro motion of dislocations with jogs producing vacancies which can condense to form voids thus nucleating a crack. This model implicitly requires diffusion of vacancies, which is strongly temperature-dependent.

4. *Loss of coherency across a slip plane due to accumulation of defects.* The basic idea of these models is the formation of configurations of dislocations in critical sites, leading to local

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