Crack stability aspects and crack growth habits in crystals

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Abstract. *In elastic-plastic crystalline solids, intrinsic/extrinsic variables affect the crack initiation and growth stages while dominating also the crack path habit. In this context, the scale factor becomes highly important with further complexities that have been related to small volume components. Comprehensive overview on fracture physics remains essential in order to develop better understanding that might reveal insights into the crack growth prediction refinements. The current study is centered on a sub-critical crack extension case in iron-based single crystals. Pre-fatigued single edge sharp crack in mini-compact specimens have been exposed to deformation/environment interaction, enhancing as such a slow crack growth that could be tracked. In fact, the current case consisted of a quasi-equilibrium crack extension, where in terms of crystal stability equation extremely tight crack stability margin prevailed. By utilizing various crack systems, anisotropic crack extension behavior was observed with significant changes of the crack front. Based on a sound background, including slip traces analysis and low energy dislocation structures, the crack-tip mechanical environment was established by a modified super-dislocation model. Simulation beside experimental confirmation defined the local crack-tip stress field by realizing plastic relaxation due to dislocation shielding. Consequently a first order approximation attributed the crack growth to the role of the fracture surface energy. Following this view point, enabled simulations to be pursued beside ultra fine features visualisation indicated consistent experimental confirmation.*

Introduction

The engagement with the crack growth habits have revealed various significant facets by adopting either microscopic (micro-structural argumentations) or macroscopic (continuum assumptions) approaches. Nevertheless, developments of local or global avenues still face a long-term challenge, namely, how the aforementioned two approaches can be bridged. For example, in terms of fracture mechanics methodology, a mixed mode situation introduces severe complexities in crack path predictions. The notion of 3D effects, dynamic-running crack vs. a semi-static situation, results in crack branching or curved paths. In this context the concept of the strain energy density criterion emerged as a dominant variable option [1-4]. Generally, the crack-tip stress field is not controlled by a single open mode stress intensity factor K_I but deserves some combination of K_m (m the specific fracture mode) might be required. As already mentioned the volume strain energy density that has been proposed by Sih [1,2] facilitated some means in order to resolve not only the fracture criterion but also the crack growth direction, as suggested for example to uniaxial crack extension of an inclined crack. The volume strain energy density theory introduced relevant hypotheses in order to propose criterion for non-self-similar crack growth situations. In this framework the partition between distortional and dilatational strain energy recognizes the mechanical damage to be either deformation or fracture, namely two processes that are inseparable. Thus, the total strain energy density describes the material damage in a global sense [1,2]. An alternative way to demonstrate some of the aforementioned concepts is formulated also by following the fracture mechanics (FM) methodology. Considering linear FM the driving force and the resistance are given by;

$$G = 2\gamma \tag{1}$$

Where the driving force G is the elastic strain energy released rate and γ is the fracture surface energy (in fact, the only resistance component in the elastic formulation). However, in this crack stability equation the interwoven relationship between the driving force and the resistance becomes apparent. Particularly by following local approach, the two critical components in the crack stability equation namely, the driving force and the resistance are clearly inseparable (once again). Some of the relevant argumentations regarding this issue are now briefly mentioned. First, experimentally based dislocation emission at the crack-tip is shaping the process zone mechanical environment. As such, the effective surface energy is dramatically affected and in mutual fashion affects the driving force. Here to mention that the strain energy density factor has a singularity of r^{-1} with directional dependency, alluding to a possible criterion that enables to predict the crack growth path. Still, notice the singularity nature of the proposed field, where r is the radial distance from the crack initiation and failure site. The FM methodology or the strain energy density approach emphasizes mainly the driving force in the crack stability equation. As known, in case of dynamic running crack, the crack extension results in crack path branching. The physical argumentations in resolving this behavior is involved and remain controversial so typical to comprehensive understanding at cases that include inertia contribution [3,4]. Even by following such methodologies fracture path criterion becomes more involved as for example in the embedded elliptical planar crack case [5-7]. In this example, the physical meaning of the critical stress intensity factor and the critical elastic strain energy release rate concepts are no more equivalent. The crack front affects also the crack stability, influenced as such by the microstructure as in duplex structure or composite systems. In addition, the crack stability issue becomes important with specific gain to be achieved in terms of the fracture resistance by crack shielding. The current study is centered on deformation/environment interaction case that enabled to explore insights as related to the role of the fracture resistance. Theoretical simulations in highly characterized systems are described and carefully observed.

Material and experimental procedures

Deformation/hydrogen interaction study selected Fe-3%wtSi single crystals in one atm gaseous hydrogen to be tracked in terms of crack stability. Sustained load tests were performed by utilizing mini-disc compact tension, pre-cracked specimens at ambient temperature. Generally, fracture mechanic methodology was used with fatigue pre-cracking, compliance calibration and exact orientation, determined for various crack systems. In order to examine the slip behavior with respect to the orientation slip trace analysis has been conducted. By following slow loading procedure beyond local yielding, slip traces were revealed by light and Scanning Electron Microscopy (SEM) visualization. Sustained load-hydrogen interaction tests were performed on {001} <100> and {001} <110> oriented specimens resulting as such in enhanced crack growth. Under the current conditions, substantial crack growth occurred that enabled assessment regarding the anisotropy factor in the crack propagation process. In addition to the external hydrogen study, internal hydrogen gaseous charging was performed. In such situations, embedded flaws expanded in a sub-critical fashion, providing information on 3D crack front behavior. Acoustic Emission (AE) tracking, Transmission Electron Microscopy (TEM) and Selected Area Channeling Patterns (SACP) assisted by SEM were also supplemented.

Computational and simulation procedures

The local approach requirements attempted to define the role of crystal plasticity. This, by affecting not only the stress state near a crack but also the slip behavior associated with the current iron-based, BCC single crystals. Thus, crack-tip slip trace analysis was conducted. Here, three dimensional finite element model was developed in order to explore the preferred operating slip systems, recognizing the triaxial stress distribution at the crack tip vicinity [8]. Beside plasticity onset, a simulation procedure with a modified super-dislocation model attempted to define the crack-tip local stress field.

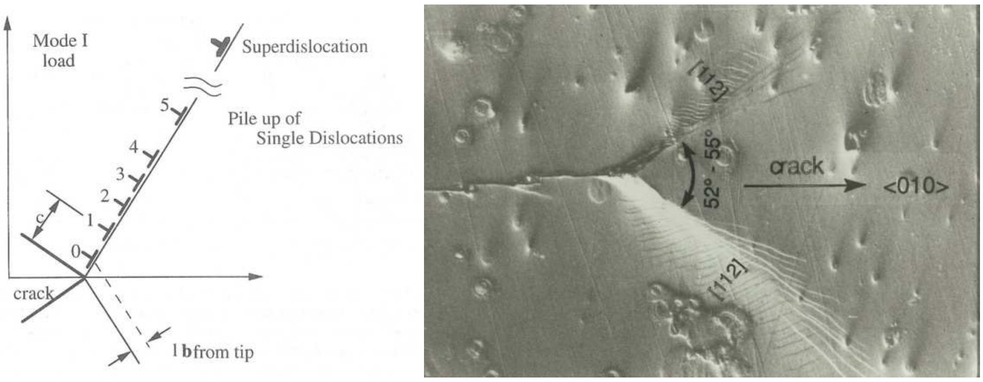

Figure 1. (Left) Modified super dislocation model (Right) Subcritical crack extansion in Fe-Si single crystal K_I=20MPa $m^{-1/2}$, crack system {001}<110>

This was an adaptation of the model proposed by Atkinson and Clements [9], simulating the plastic relaxation ahead of the crack-tip, associated also with the dislocation shielding effects. Recognizing other argumentations it seems worthwhile to examine local stress field variations due to crack extension or its specific effects on the arrest potential [10]. Finally, the crack or a flaw front analysis was assisted by surface energy effects - generation of the Gibbs-Wulff construction that became also a relevant method engaging with a macro cleavage plane case. In extremely small margin case in terms of the crack stability conditions, deformation/environment case served to demonstrate the crack extension to be a surface energy controlled with directional dependency process.

Experimental, computational and simulation results

Surface slip traces for three crack systems orientation demonstrated that predominant slip system to be {110}<-111>. This occurred at earliest stage of yielding in contrast to multiple slip that developed at higher levels of K_I. Typical mechanical properties for <100> at ambient temperatures and 10^{-3} strain rate indicated yield strained and work hardening exponent of 300MPa and 0.38 respectively. More to mention, that slip bends were intimately connected with 1μm spaced arrest-lines that were observed fractographically and acoustically. The crack-tip trace analyses indicated that the theoretical prediction and the experimental findings are in a strong agreement, which strengthens the crack-tip morphology characterization as described. The elastic-plastic dislocation model simulations treated three variations of dislocation arrangements. The basic idea here was in screening possibilities that might lead to maximum stress modifications. Physically, this might result by activating secondary dislocation sources at an early stage of crack propagation. Following such micro process, a crack jump forward by one micro-structural unit (about 1 μm) becomes possible. By extending the stationary situation to the aforementioned quasi-static dynamic process, the maximum stress peak drops down (estimated by the simulation to a drop down of 6000 MPa). Even by ignoring the role of the environmental agents and its critical concentration aspects, such significant decrease of the stress ahead of the crack-tip might be enough to slow down the crack or even arrest it. Actually, this suggests a possible role of a diminished driving force aiding arrest. Clearly the decrease of the driving force might be in conjunction of plasticity or the directional features of the fracture surface energy. The latter is associated with the resistance component in the crack stability equation. Finally, consider the crack front and the void shapes as being primarily a surface energy controlled process. For example, the [001] zone axis is illustrated with the appropriate Gibbs-Wulff plot and the corresponding Gibbs-Wulff construction.

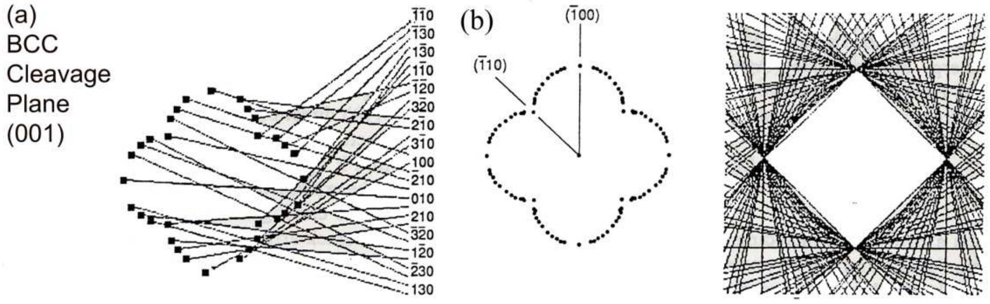

Figure 2. (Left) Gibbs-Wulff construction W(u) (Right) Flaw crack path-G(u) for {001} zone axis

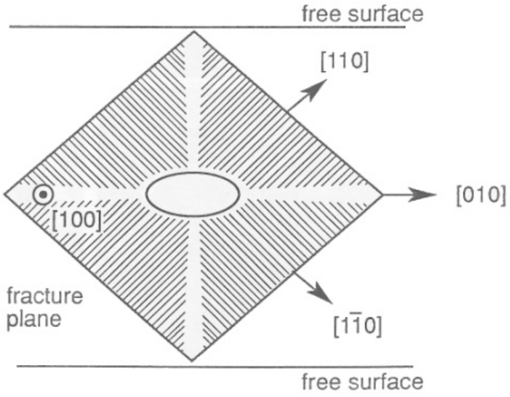

Figure 3. Schematic crack extension

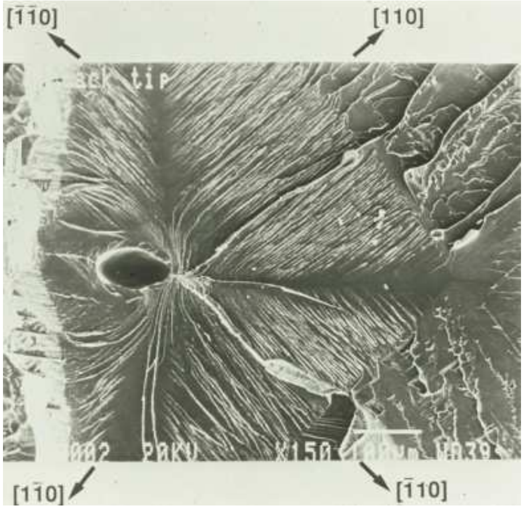

Figure 4. Observed crack extension due to internally deformation/hydrogen interaction, crack front along <110>

Generally the analysis applied to both, the crack front developed from a compact tension pre-fatigued specimens. Regardless if internal or external environment, although the embedded internal flaw applied clearly to the internal hydrogen case. As demonstrated the comparison between the simulated crack extension shape and the experimental observation regarding the crack front is striking. The anisotropic features are readily observed, indicating a different shape than originally predicted by Ayres and Stein that involved favorable <100> growth direction [11]. Although substantial attention has been given to the anisotropic role of the effective surface energy, there is no intention to de-emphasize the localized and directional aspects of the driving force. It appears that the local approach as related to the driving force, makes the anisotropic nature of the driving force, as well, more conceivable. The emphasis of the driving force motivated the current investigation to engage with the resistance as dominated by crystal plasticity and thus, inherently associated with anisotropic behavior.

Discussion, summary and conclusions

The study touches findings as related to enhanced sub-critical slow crack growth on a micro cleavage plane. Such crack extension occurred by deformation/environment interaction. Based on crack stability considerations further insights included initiation/arrest behavior, crack front aspects and directional crack extension habits. Some of the questions are why the discontinuous micro-process prefers specific <110> directions and why different levels of semi-brittle fracture modes are associated with environmentally-induced cracking. In order to understand these, it is first important to recall the stress distribution as described by the dislocation model for this well-defined crack-tip morphology. Here, a very high stress is achieved about 20nm in front of the crack-tip. It has been shown [12] that corresponding hydrogen enrichment and local decohesion is possible due to micro-cleavage triggering of the {100} cleavage planes. Based on our observations of initiation patterns, it is proposed that these are actually isotropic in nature. If then the local resistance is extended in scale, the meaning of the effective surface energy becomes apparent. Since slip bands are intersecting at the cleavage plane, they provide an anisotropic resistance to crack extension. Therefore directional features are left on the fracture surface in the wake of the traveling crack. The proposed chain of events has been based on experimental evidence from surface slip surfaces, TEM and acoustic emission tracking. Similar to the early work by Mullins and Sekera [13] and Y.Katz et all [14] which dealt also with dislocation configurations in anisotropic media. Generally, one can draw a surface W(u) representing the variations of the energy W with the orientation u by following this, A Gibbs-Wolff construction G(u) that can be generated formed by the inner envelope of the Plaines normal to the vector u. For example, two crack systems resulted in different crack path and fronts in one case, straight crack front prevailed compared to two orthogonal zigzag crack front that was observed consistently for the second. Finally, further elaboration concerning the scale effect and the material characterization is now in order. Still, in the elastic FM framework, consider an embedded planer elliptical sharp crack. This crack represents a non uniform stress intensity factor around the crack border. Here, the exact quantitative evaluation of crack stability depends on the crack path habit [14,15]. Accordingly the following is concluded.

1. The anisotropic nature of the local crack stability is manifested in BCC semi-brittle crystals. Enhanced crack extension due to deformation/environment interaction indicated the role of the directional dependency of the effective surface energy.
2. Regardless if either local or global approaches are adopted the notion that plasticity and fracture are inseparable still prevails.
3. In the current quasi-equilibrium crack extension theoretical simulation based on solely effective surface energy controlled mechanism have been confirmed.

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