Plasticity, a Major Agent in Triggering a Brittle Fracture Mode

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Abstract. The current study elaborate on two theoretical/experimental based interactive cases that provided additional input into fracture mode transition events. First, iron-silicon single crystals were selected for basic investigation under deformation/environment interaction. Second, micro-crack stability aspects that have been assisted by load interaction effects in polycrystalline and single crystal systems. In order to gather deductive information, novel techniques were utilized in the framework of a combined measurements/visualization program. Physical insights into the dynamic nature of the sub-critical crack regime have been developed. Topics as related to crack-tip shielding, crack initiation and arrest potential were assisted by crack-tip dislocation emission model. Specifically, the discontinuous crack extension on the macro cleavage plane in a ductile/brittle transition pattern remains striking, specifically concerning the critical role of local plasticity.

Introduction

Extensive volume of research activities have been invested the current topic, forming as such a full and a self-contained discipline. For decades, the material response in terms of displacements and structural integrity has remained a major concern. However, from the thick forests of information and only as a reminder, illustrations of early works on cleavage are singled out [1,2]. Generally, there is the tendency to examine crack stability in terms of a balance between the driving force and the fracture resistance. If ideal elasticity is considered the crack stability equation is given by:

$$G = 2\gamma_i \qquad (1)$$

Where; G is the elastic strain energy release rate and γ_i is the intrinsic surface energy for fracture. In fact, in a given reversible response, the surface energy is the only resistance component by following either the stress field analysis or adopted thermodynamic energy argumentations. Initially, crack stability variables have been expressed by global continuum theory, describing mainly the process end result, eventually, with limited description of the sequential micro-mechanisms that are involved in the fracture process. Thus, in terms of a comprehensive viewpoint, the crack formation and extension does not adhere to the mathematical sense of the crack stability equation. Notice that, the driving force and the resistance have higher order of secondary mutual effects in a kind of interwoven fashion. Local crack-tip environment affect the driving force and dislocations emission dominate the effective surface energy. It became apparent that only by adopting a local approach, refinements could be explored as related to the dominating components of the crack stability equation. Following a discretized crack-tip dislocation emission model micro mechanisms of brittle fracture were rationalized beside experimental conformation. The model has been extended to deformation/hydrogen interaction case that offered significant input of computation beside experiment finding levels in a systematic and consistant methodology. Again, for the first case, namely sub-critical crack extension of iron-silicon single crystals enabled to be engaged with topics concerning anisotropic crack extension, crack-tip shielding, arrest potential vis-à-vis crystal plasticity and slow crack growth on a macro cleavage plane. The issue of crack initiation and arrest potential are characterized also by the Pop-In (PI) phenomena that was selected as a second case. Here the study demonstrates additional findings like the case of overload in which the pop-in is consistently affected and eventually diminished. Here, two fronts have been recognized. First, the tracking of local crack extension bursts, namely the PI occurrence. Second, the characterization of the local fracture mode dominated by the PI event. The study incentive emerges from the notion that the driving force and the resistance are not separable by nature, currently demonstrated by two examples. The connectivity between the global stress intensity and the critical Griffith value has been modeled by the aforementioned organized-discreitezed dislocation simulation. Single dislocations represented the near tip distribution while a super-dislocation represented the far-field plasticity (Figure 1)

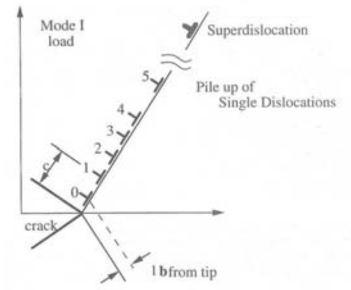

Figure 1. Crack tip dislocation emission

By numerical computation using anisotropic elasticity theory the equilibrium positions of all dislocations could be established. Moreover, the local crack tip stress intensity factor and the stress field distribution could be specified. Recognizing this framework, systematic experimental program was conducted in order to confirm the feasibility of the proposed approach. The adopted term from mineralogists, namely, cleavage, in typical crystal structures confined to specific crystallographic planes. In the fracture field classical dilemma have been related to B.C.C. transition metals that encourage dislocation models associated with the brittle mode of fracture [3-5]. By definition dislocation based models alluded to the significant role of plasticity in triggering brittle transitions. Thus, local approach anchored by multi-scale simulation, accentuated the role of plasticity in triggering brittle fracture.

Materials and experimental procedures
Iron-based single crystals

Single crystals of Fe-3wt%Si were selected, received as bars of <010> and <110> direction axes. X-ray, back reflection Laue, assisted in establishing their orientation. Beside determination of constitutive mechanical properties, fracture mechanics methodology test were supplemented. Thus, miniature disc shape, pre-fatigued, single edged notch specimens in the rage of 0.9 to 4.8 mm were used. Careful attention was paid to the cold machining processes in order to minimize prior specimen damage. Due to difficulties at this stage in controlling the crack stability or even integrity, the pre-fatigued crack sharpening was conducted under compression-compression conditions at 150 K. This resulted in extremely sharp crack-tip that has been extended at ΔK=25 MPam$^{1/2}$ and a load ratio of R=10. Crack orientations of {001} <010>, {001} <110> and {011} <011> were studied in order to resolve the directional dependency (see Figure 2).

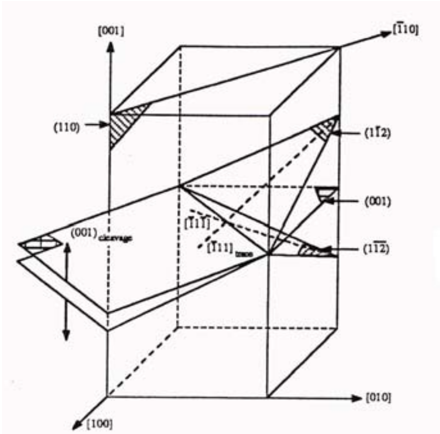

Figure 2. Crack system {001} <110

Internal and external hydrogen were introduced to allow unstable circumstances of deformation/environment interaction. Such interaction affected crack stability that could be tracked, measured and visualized. Thus, the sub-critical crack extension regime was achieved either by sustained load or cyclic loading. Standard mechanical properties like yield, ultimate stresses and strain-hardening exponents were established using closed looped electro-hydraulic set-up at ambient temperature.

Concepts	**Framework**	**Observations**	**Analysis**	**Objectives**
Local and micro mechanics approach	Deformation/environment interaction and external/internal subcritical flaw/crack growth in single crystals	Crack-tip enclave-slip traces	Finite element analysis	Crack-tip morphology characterization following crystal plasticity
			Elastic-plastic numerical simulations	Microcrack growth/arrest Driving force with reflection on the local resistance
		Fracture morphology crack front or void shape	Gibbs-Wulff plots and construction	Semi-equilibrium stabilization trends local resistance aspects with reflection on the local driving force
		Crack initiation and propagation stages	Fracture mechanics considerations	Anisotropic aspects, structure modes transition

Table 1. Crack stability-comprehensive program

For this purpose, uniaxial tensile specimens were utilized at a rate of $5x10^{-3}$ sec^{-1}. The crack-dislocation interaction was characterized also by establishing dislocation structures, namely beside low energy structure the distribution and position relatively to the crack-tip was supplemented. This experimental section was achieved by Transmission Electron Microscopy (TEM). In addition, slip trace analysis was performed by light and Scanning Electron Microscopy (SEM) that contributed also to Selected Area Channeling Pattern (SACP) that was performed on the fracture plane. By channeling, lines width and the relative sharpness are affected by the near surface strain enables as such the assessment of local plasticity. Additional information resulted from Crack Opening Displacement (COD) gage that established the crack-tip position (in case of crack extension) and the elapsed time that enabled to determine velocities in high resolution. The latter information was completed by Acoustic Emission (AE) technique referring to the question of the crack advancement nature and characterization. More of the detailed program is given in Table 1.

Pop-in polycrystalline systems

Construction materials like steel and Aluminum alloys were selected. Standard mechanical characterization was conducted including the determination of fracture mechanics parameters. Tests were performed by using closed loop electro-hydraulic machines for constitutive properties and fracture mechanics parameters information. For the latter, temperature range between 77 to 296K was screened for different loading rates. Three points bend specimens were used with pre-fatigued single edge notched geometry and initial crack length of 2mm. Specimen dimensions were 10x10x55 mm and the pre-fatigue and the final fracture tests were performed at the same temperature. The selected rate and stroke controlled conditions were in the rates between 0.62 to 300 mm/sec. Besides the load response recording, COD and AE signals were monitored simultaneously in order to match the load tracking. The PI velocity was measured by electro-potential technique supplemented with appropriate software. For materials characterized by ductile-brittle transition, tests included also the lower shelf regime with and without Warm Pre-Stressing (WPS) effects. Fracture mode observation at the PI zone included also chemical classification, namely in order to reveal the possible role of metalloids affecting crack stability. The AE events were screened during monotonic loading with attention to wave emission associated with PI occurrence. Finally, optical and SEM were utilized for fracture mode transition classification at the PI zones and the unstable crack extension regime.

Experimental results

Iron based single crystals with environmental interaction

For the selected Fe-3wt%Si crystals mechanical properties were conducted. At ambient temperature, and relatively low crosshead rate of 5×10^{-3} sec^{-1}, yield stress of 300 MPa with modulus $E_{[100]}$ 1.33×10^{5} MPa, and strain hardening exponent n=0.38 values were established. In terms of fracture mechanics parameters, the critical stress intensity for cleavage in the Griffith crack is;

$$K_{IG} = \left(\frac{E\gamma_i}{1-\nu^2}\right)^{\frac{1}{2}} \tag{2}$$

Where; E is the Young's modulus γ_i the ideal surface energy for fracture. Clearly, crack-tip dislocation emission, affects in a complex fashion both the driving force and the resistance. The interaction with hydrogen for sustained load tests enhanced also a sub-critical crack extension. For crack extension rate of about 5.10^{-8} m/sec it became apparent from slip trace analysis, dislocation arrangements ahead of the crack tip and SACP information that the brittle mode is accompanied by significant plasticity. The complex experimental program in the current semi-brittle crystals and environmental interaction enabled to have the required resolution in order to establish the local alternating ductile/brittle transition occurrence. Due to small margins in the crack stability a step wise behavior occurred. A stage of certain stability is achieved on one hand by dislocation emission shielding but on the other, locally, micro-cleavage is enhanced by hydrogen interaction. Based on fractography and AE the sub-critical crack extension on the macro cleavage plane was discontinuous. This complex slow crack growth process followed a consistent chain of events, namely crack initiation, arrest and reinitiating. These important insights have been elaborated elsewhere.[6-9]. The complex cleavage issue followed argumentations by Rice and others [6,10] have been currently supplemented by ultra fine features observation including dislocation densities and distribution analysis. The Atkinson and Clements formulation [11] developed a super-dislocation model for the crack-tip dislocation emission analysis. In this context, the super-dislocation approximation model proposed some advantages over the continuous dislocations array model. With the assistance of numerical computation mechanics the local crack-tip stress field for open mode loading system was attempted quantitatively. The efforts of experimental matching revealed the model key-point, namely, to be highly relevant and physically based model.

The pop-in events

For the sake of briefness, the findings as related to the AISI 4340 system are mainly described. Monotonic loading as performed on pre-fatigued specimens has revealed typical mechanical responses. Even at the Hookeian portion of the load-displacement curve, the AE activity has been detected prior to the first PI event. Wave emission groups were analyzed in terms of energy distribution and time factors. Although the PI was extremely sudden, the crack extension within the area swept by the PI event remained discontinuous with typical low energy fracture surface classification. Constitutive variables that affect the flow behavior influence strongly the PI trends. Here, the study was centered on the thermal and the strain rate dependency. In the range of the current investigation imposed rates of five orders of magnitude resulted in average pop-in velocity changes of two orders of magnitudes. Fractographic findings indicated in AISI 4340, enhanced cleavage associated directly to the PI phenomena. Exploring the macro PI events emphasize the role of various factors like the state of stress that affect surface plasticity. In this context, ligaments beside intrinsic driving force/resistance margins are enough origins in enhancing the localized sub-critical crack initiation and arrest. The effects of WPS is illustrated in Figure 3.

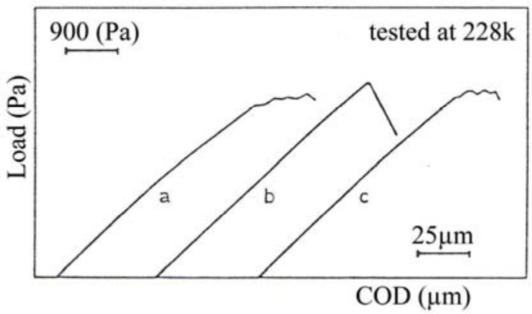

Figure 3. PI affected by WPS (a) with no WPS (b) with WPS (c) after relaxation

Discussion

Crack system orientation resulted in variations of the dislocation arrangements due to crystal plasticity. Following the elastic-plastic dislocations emission model, the simulation indicated the variations of the localized crack-tip maximum stress values that are clearly expected. For example, as addressed elsewhere [10] the stress peak could drop down by as much as 6000 MPa by examining solely the role of dislocation arrangement, even by ignoring interactive agents. This raises the option that significant decrease of the stress ahead of the crack-tip might be enough to slow down or even arrest the crack. Thus, the notion here suggests the possible option of diminished driving force aiding arrest in conjunction with plasticity or the directional feature of the surface energy. The latter is clearly associated with the resistance component in the crack stability equation manifested by findings that different crack orientation affected also the advancing crack front. The {100} <011> crack system resulted in a straight local crack front along a <011> direction. This in contrast to {100} <010> crack system in which a zigzag crack front was established along two orthogonal <011> directions. Although substantial attention has been given to the anisotropic role of the effective surface energy, the role of the localized and directional aspects of the driving force remained significant. More aspects regarding the anisotropic behavior have been addressed by Katz et al [12]. The striking point of the study is centered on the crack arrest in contrast to the crack growth increment. This has been concluded by observed habits of the sub-critical crack extension. Again, this is accepted as a major point to support the arrest potential available in semi-brittle crystals. A major advance in the understanding of crack instability in semi-brittle materials was the Rice and Thomson concept [6] that was later applied to environmental degradation with surface energy arguments [12]. The marginal stability depends on whether the conditions for dislocation emission or cleavage in the Griffith sense are achieved (see Figure 4).

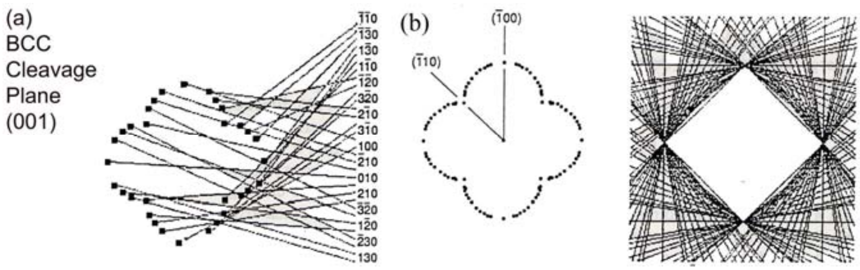

Figure 4. a&b Gibbs-Wulff plots and construction

Local stress intensity for dislocation emission, K_{Ie} in open mode is given by:

$$K_{Ie} = \frac{\mu b}{\sin\alpha \bullet \cos\frac{\alpha}{2}\{2\pi r_0(1-\upsilon)\}^{\frac{1}{2}}} \tag{3}$$

Where; r_0 is a core radius including the crack-tip and a dislocation loop, μ is the shear modulus, υ the Poisson ratio and α the angle between the crack and the emission plane. For the Fe-3%wtSi selected crystals, K_{Ie} and K_{Ic} are between 0.7 and 1.4 MPa in ½, implying that either ductile or brittle behavior maybe exhibited in this borderline system. The aforementioned borderline behavior has been shown also by 3D crack, molecular dynamics simulation [13]. For the current BCC iron based crystals the N-body potentials of Finnis-Sinclair type was applied in order to reveal the mechanical response by thermal conditions.

The PI phenomena have been attributed also to micro-structural heterogeneity either segregation elements or local phases morphology. Phases distribution might include also inversion under localized stress field. Nevertheless, the discontinuous behavior of static or running crack is not unique only to crystalline systems. For examples, the pop-in mode occurrence has been addressed earlier by Key and Katz in polycarbonate glossy polymer [14]. The linkage to plane stress or strain conditions is argued beside other proposals attributing the mechanical response to polymer relaxation properties [15]. In practical sense, the PI events are well expressed in the standardization of fracture toughness parameters. In order to extend the understanding regarding the macro PI phenomena Warm Pre-Stressing (WPS) conditions were finally included in order to assess the role of elastic stored energy surplus on the PI phenomena. This experimental section became beneficial, contributing to the marginal concept in the crack stability equation. In fact, with the corporation of WPS, the PI diminished consistently like in blunt vs. sharp crack-tip. The domination of the aggressive environment provided appropriate conditions to explore additional facets of the crack behavior. The meaning here is to enjoy input under extremely narrow marginal situation between the driving force and the resistance.

Summary and Conclusions

The anisotropic nature of the local crack stability is manifested in BCC semi-brittle single crystals. The coupled driving force-resistance components complicate the fracture physics as observed on a macro cleavage plane. Dislocation arrangements or rearrangements alone might reduce the driving force. As such, any crack hesitation will enhance the local effective surface energy in terms of dislocation dynamics alone. The study under deformation/environment interaction has determined the shape of the crack front on a given cleavage plane. Accordingly, the following are concluded:

(1) Assisted by deformation / environment circumstances and iron-based single crystals the role of plasticity in the extension of a sub-critical cleavage has been manifested.
(2) Experimental confirmation beside crack-tip dislocation interaction model has offered further insights as related to the sub-critical slow crack growth situation.
(3) The study of highly localized crack instability becomes beneficial in developing physical-based elements into the fracture process.
(4) The mutual interaction between the fracture resistance and the driving force suggests that a generic crack stability equation governs in a coupled fashion the fracture event.

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