Three-dimensional analysis of mesoscale deformation phenomena in welded low-carbon steel

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A three-dimensional numerical analysis of the mesoscale deformation behavior of welded low-carbon steel specimens is performed. A weld-affected polycrystalline microstructure is designed to reproduce gradual changes of the grain size throughout the base metal and heat-affected zone regions. A mathematical model based on a double-limit yield criterion is used to describe Lüders band propagation characteristic of this type of steel. The effects of the free surface, grain boundaries and interfaces between the fusion zone and the heat-affected zone, and between the heat-affected zone and the base metal are discussed.

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1. Introduction

Engineering predictions of the deformation and fracture behavior of welded structures are commonly based on the estimation of macroscopic characteristics (static, dynamic and fatigue strength, macroscopic yield stress, etc.). In actual fact, welded specimens are characterized by a wide variety of interfaces of different scales and configurations which give rise to stress concentration at micromeso- and macroscales [1–7]. A thorough study of the multiscale phenomena in welded materials takes on special significance because a gradual accumulation of irreversible deformation and damage at lower scales may lead to macroscopic failure of the welded structure.

An inhomogeneous stress–strain state on the macroscale is controlled by the shape of the weld, geometry of the welded specimen and variation of the mechanical properties throughout the base metal – heat-affected zone (HAZ) – fusion regions. It was found experimentally [5–7] that the interfaces between the fusion zone, HAZ and base metal were responsible for the nucleation of localized shear bands and for subsequent fracture of welded specimens. The microstructure, in its turn, is responsible for stress concentration and plastic strain localization at a lower scale in microregions of the material. Experimental and theoretical studies (e.g., [8–12]) showed that microscale stresses and strains are scattered about macroscopic (mean) values. Estimations of the local microstresses and strains are important, e.g., for fracture predictions under fatigue loading. The external forces under fatigue are typically so small that the average stress–strain response does not exceed the elastic limit of the material. In the vicinity of interfaces (e.g., grain boundaries), however, the microscale stresses and strains are redistributed, with their values oscillating about an average level. The stress concentration may induce local plastic deformation and ensuing microcracking. Development of methods for optimizing the microstructure and properties of welded joints to minimize a hazardous stress–concentration level near the interfaces is an acute engineering and scientific problem that calls for theoretical and experimental investigations.

In our earlier work [13] we performed a three-dimensional numerical simulation of the deformation behavior of macroscopic welded steel specimens under tension. The base metal, HAZ and fusion zone were distinguished by their mechanical properties and the interfaces between the three regions were assumed to be plane. The analysis focused on the estimation of the macroscale stresses and strains. In this paper the macroscopic analysis is complemented with microstructure-based simulations with an explicit account of weld-affected microstructure.

2. Experimental background

Extensive experimental data on the deformation and fracture behavior of a welded low-carbon steel simulated numerically in
this paper are presented in [5]. Welded specimens consisted of three distinct regions: fusion zone, base metal and heat-affected zone (HAZ). The latter two regions are characterized by polycrystalline ferrite microstructure (Fig. 1(a)), with grains in the HAZ being half as large as those in the base metal (i.e., 8 and 15 μm). The mechanical properties of the HAZ and base metal were obtained indirectly from microhardness distributions throughout the weld-affected material [5]. The microhardness in the fusion zone was reported to be 30% higher than in the base metal, and the elastic-plastic properties were assumed to vary proportionally.

According to [5], plastic deformation and crack nucleation and development take place in the HAZ and in the base metal, but these processes never occur in the fusion zone or in the adjacent overheated regions of the HAZ. Three basic stages of plastic deformation in the welded steel specimens were revealed and examined. The first stage is characterized by formation of mesoscopic shear bands evident as Lüders bands. The mechanical properties of the HAZ and base metal were obtained indirectly from microhardness distributions throughout the weld-affected material [5]. The microhardness in the fusion zone was reported to be 30% higher than in the base metal, and the elastic-plastic properties were assumed to vary proportionally.


g is the bulk modulus. The stress deviator and strain tensor components εij and δij and the yield criterion describing the elastic-plastic transition.

The stress tensor components σij are expressed in terms of the sum of hydrostatic and deviatoric parts to get

\[
\sigma_{ij} = -P\delta_{ij} + S_{ij}
\]

where \(P\) is the pressure, \(S_{ij}\) is the stress deviator components, \(\delta_{ij}\) is the Kronecker delta and the dots designate the derivative with respect to time. To describe the hydrostatic part of the stress tensor under quasi-static loading, it is expedient to make use of the following linear equation of state

\[
P = -K\varepsilon_{kk}
\]

where \(K\) is the bulk modulus. The stress deviator and strain rate deviator components for an elastic-plastic medium are given by the relation

\[
\dot{S}_{ij} + \lambda S_{ij} = 2\mu \left( \dot{\varepsilon}_{ij} - \frac{1}{3} \dot{\varepsilon}_{kk} \delta_{ij} \right)
\]
where \( \mu \) is the shear modulus. The scalar factor \( \lambda \) is identically zero in the elastic region and is nonzero in the region of plastic flow. The strain rate tensor is expressed by a relation of the form

\[
\dot{\varepsilon}_{ij} = \frac{1}{2}(U_{ij} + U_{ji}) = \dot{\varepsilon}_{eq}^e + \dot{\varepsilon}_{eq}^p
\]

where \( U_{ij} = \dot{x}_i \) is the velocity vector, \( \dot{x}_i \) is the spatial coordinates, \( \dot{\varepsilon}_{eq}^e \) and \( \dot{\varepsilon}_{eq}^p \) are the respective elastic and plastic strain tensor components, the commas denote the derivative with respect to the corresponding coordinate.

A characteristic feature of the examined steel is the development of plastic deformation evident as Lüders bands [15,16]. To take into account this phenomenon, use was made of a double-limit yield criterion based on the experimental data on the dislocation behavior of this type of steel. The experimental evidence obtained in [15] shows that dislocations originally present in the bulk of the material, as a rule, are immobilized. The detachment of dislocations and the nucleation of new defects capable of plastic flow initiation require a higher stress level than the one at which subsequent propagation of dislocations takes place. This kind of model underlies the double-limit yield criterion written in the following form:

\[
\sigma_{eq} = \begin{cases} \sigma_t & \text{if } \varepsilon_{eq}^p = 0 \\ \sigma_t(\varepsilon_{eq}^p / \varepsilon_{eq}^p) & \text{if } \varepsilon_{eq}^p > 0 \end{cases}
\]

where \( \sigma_t(\varepsilon_{eq}^p / \varepsilon_{eq}^p) \) is the strain-hardening function. Two yield limits are introduced in the von Mises yield criterion: a higher stress (triggering stress) \( \sigma_t \) is necessary to initiate plastic flow in an elastically strained material and a lower stress (yield stress) \( \sigma_t \) is required to maintain plastic deformation in these regions. In other words, once a local region in the material is transformed from an elastic into a plastic state, there is an abrupt drop in the yield stress followed by plastic deformation at a lower stress level.

The double-limit criterion was used in [13] to simulate the evolution of Lüders fronts in welded and unwelded low-carbon steel specimens. This criterion in combination with an appropriate strain-hardening function was shown to provide an adequate description of Lüders band propagation. A representative illustration for the unwelded specimen is given in Fig. 3. The Lüders fronts are formed near the fillet rounding regions, which corresponds to a yield drop in the macroscopic stress–strain curve (Fig. 3(a) and (b)). Then the Lüders bands start to counterpropagate along the specimen at an approximately constant velocity proportional to the macroscopic tensile strain (Fig. 3(c)). This is represented by a horizontal portion of the stress–strain curve (the Lüders plateau). The plastic strain rate is at a maximum in the fronts and is nearly zero behind them. Once the entire specimen is involved in plastic flow (Fig. 3(d)), the stress–strain curve reaches the strain-hardening stage.

### 3.3. Microstructure, mechanical properties and loading conditions

The first step in the development of a material model implies the design of a three-dimensional microstructure. To generate microstructure of the examined welded steel, use was made of a step-by-step packing algorithm considered at length in [12]. As initial conditions, a rectangular volume was discretized by a regular cubic mesh of \( 220 \times 100 \times 50 \) and grain nuclei were distributed over the base metal and the heat affected zone in the ratio 1:3 to reproduce a gradual change in the grain size throughout these regions. A subsequent grain growth obeys a spherical law, with the growth rate being the same during the growth process. The resulting polycrystalline model is presented in Fig. 4(a). Grains in the HAZ are about half as large as those in the base metal (Fig. 4(b)), as observed in [5]. Following the experiment-based assumption that the material in the fusion zone is plastically undeformable, the microstructure of this region was disregarded from explicit consideration.

Polycrystalline grains in the base metal and HAZ were distinguished by their elastic-plastic properties. In a general case, elastic and plastic properties of individual grains are controlled by their crystallographic orientation with respect to load. In many works (e.g., [9,10,17,18], grain orientation was accounted for through the Hall–Petch relation

\[
y = y_0 + k_s \sqrt{D_i}
\]

where the upper index \( i \) is the grain index. The initial yield stress \( \sigma_0^i \) of the \( i \)th grain is related with the grain size through the Hall–Petch relation

\[
\sigma_0^i = \sigma_t + \frac{k_y}{\sqrt{D_i}}
\]
where $\sigma_s = 50$ MPa is the yield stress for an iron single crystal, $k_y = 1384$ MPa $\mu m^{1/2}$ is the grain-boundary hardening coefficient (Hall–Petch constant) and $D_i^{\mu}$ is the diameter of the $i$th grain. In the numerical realization, the grain diameter was calculated as the diameter of a sphere of the same volume. According to Eqs. (6) and (7), the smaller the grain, the higher its yield limit. Therefore, for the model used (Fig. 4(a)), the larger grains in the base metal possess a higher yielding ability than those in the HAZ. The elastic-to-plastic transition obeys the double-limit yield criterion, Eq. (5). The difference between the triggering stress $\sigma_0^t$ and the initial yield stress $\sigma_0^i$ was 96.3 MPa.

The elastic characteristics of grains were assigned to provide a fit to the experimental data on microhardness distribution throughout the base metal and HAZ regions [5]. The following mean shear and bulk moduli were assigned in the calculations: $\mu_{HAZ} = 92$ GPa, $\mu_{BM} = 80$ GPa, $K_{HAZ} = 153$ GPa and $K_{BM} = 133$ GPa. The upper indices “HAZ” and “BM” denote the elastic constants for the HAZ and base metal, respectively.

The loading scheme is shown in Fig. 4(a). Tensile or compressive load was applied to the opposite ends of the specimen along the $X_3$-axis at a constant velocity. The displacements of the loaded surfaces along directions $X_1$ and $X_2$ were not constrained. The other four specimen surfaces were assumed to be free from the action of external forces.

4. Computational results and discussion

4.1. Stress concentration analysis

Due to microstructural inhomogeneity, all components of the stress and strain tensors in local microregions of a loaded material take on nonzero values. Macroscopically homogenized stresses and strains are redistributed on the microscale level and demonstrate a scatter about the mean value. Extensive experimental and theoretical studies (see, e.g., [6,8–13]) suggest that the governing factors responsible for stress concentrations near the interfaces are the difference in the mechanical characteristics between the contacting materials, the curvature of the interfaces and the loading conditions. In the model examined (Fig. 4(a)) there are several kinds of interfaces giving rise to stress concentration at different scale levels. Let us analyze their individual and combined contribution to the mesoscale deformation response. The second invariant of the stress tensor (equivalent stress) is chosen as the material response parameter independent of any coordinate system.

Referring to Fig. 5, grain boundaries give rise to stress concentration from the very onset of loading. The highest stress level is realized in the vicinity of triple junctions of grains characterized by markedly different elastic properties. With the model used, these are the HAZ regions adjacent to the base metal and to the fusion zone. While the elastic moduli of grains in the base metal are varied within 5% and so is the difference between HAZ grains, the difference in mechanical properties between the two regions may exceed 30% in proportion to the average grain diameter (see Fig. 4(b)).

The specimen free surface, in its turn, is the most powerful source of stress concentration because it serves as an interface between materials with essentially different mechanical properties (metal-air interface). As soon as load is applied the free surface being flat in a prestrained state undergoes pronounced out-of-plane displacements (Fig. 6(a)). A characteristic feature of this phenomenon referred to as strain-induced surface roughening (see, e.g., [18–20]) is that groups of grains instead of single grains are involved in a cooperative motion to form hills, hollows...
Fig. 5. Equivalent stresses on the surface (a) and in the bulk section of the welded specimen (b) at $\varepsilon = 0.1\%$.

Fig. 6. Free surface profiles in the welded steel at tensile strain of 0.1 (a), 0.5 (b) and 1.5% (c).

or folds on the surface. Under loading, the surface pattern undergoes qualitative changes, with the roughness amplitude being increased nonlinearly (see Fig. 6(a and b)). Without going into further details, we will simply note that the surface roughening makes an additional contribution to local stresses. Shown in Fig. 5 are the equivalent stress patterns on the surface and in the bulk section of the welded specimen obtained in the elastic loading stage. The scatter of local stress values is more pronounced on the surface (Fig. 5(a)) than in the bulk of the specimen (Fig. 5(b)). This is the mechanical cause of the onset of plastic deformation on the surface rather than in the bulk of the specimen.

Summarizing, we may conclude that three main sources of stress concentration (surface, grain boundaries, and HAZ-base metal and HAZ-fusion zone interfaces) acting together give rise to the highest equivalent stress level on the specimen surface in the vicinity of interfaces between the HAZ and base metal grains and between the HAZ and the fusion zone.

4.2. Plastic flow

Let us compare plastic strain patterns in Fig. 7 with the macroscopic stress–strain curve in Fig. 8, where $\sigma$ is the overall stress and $\varepsilon$ is the overall tensile strain of the specimen. Although the highest

Fig. 7. Plastic strain patterns at an overall strain of 0.2 (a), 0.3 (b) and 1.0% (c).
local stresses are realized in near-boundary HAZ regions, the early plastic strain takes place in the base metal whose grains are more prone to plastic deformation. As predicted by the stress concentration analysis, plastic flow appears initially in surface grains located near the loaded end of the specimen and progressively covers the entire section of the specimen, forming the Lüders band front (Fig. 7(a)). Accordingly, the descending branch of the stress–strain curve (Fig. 8) demonstrates a drop part (the yield tooth) in agreement with experiment.

On further loading the LB front starts to propagate along the specimen toward the weld-affected region (Fig. 7(b)). This process corresponds to the Lüders plateau in the curve (Fig. 8). The band propagation is controlled by competing processes of plastic strain nucleation ahead of the front and strain hardening behind it. The LB front itself can be treated as a peculiar kind of the interface between the elastically and plastically strained regions. The LB velocity varies for grains with different yield ability. Thus, the LB front at the microscale is not a rectilinear interface but acquires local curvature responsible for the additional increase in local stresses in the elastic material ahead of the front. As the LB reaches the imaginary interface between the base metal and the HAZ, it ceases to propagate, which corresponds to the early strain-hardening portion of the stress–strain curve. For examined degrees of strain, further plastic deformation localizes entirely in the base metal. We believe, however, that the HAZ regions also may be involved in plastic flow at a later loading stage where the yield characteristics in the base metal increase due to strain-hardening.

Since the microstructure under study is not representative, the calculated stress–strain curve deviates from experiment in the Lüders deformation stage, i.e., in the calculations the yield tooth is 20% higher and the Lüders plateau is shorter because the plastic deformation front covers a shorter distance.

### 4.3. Fracture prediction

A great body of experimental and theoretical data (see, e.g., [21–26]) suggests that pores, voids and microcracks nucleate and develop in positive triaxial strain regions $\varepsilon_{kk} > 0$. Thus, for the purpose of fracture prediction it is important to analyze triaxial stress and/or strain patterns. From the viewpoint of classical macroscopic mechanics, positive triaxial strains in a homogeneous isotropic material arise in limited cases, e.g., under tensile loading, whereas in compression all points of the material undergo negative bulk strain. In the latter case, the proposed model for crack nucleation in triaxial tensile regions breaks down. For inhomogeneous materials, however, the model for fracture initiation in the positive triaxial strain regions provides an adequate description of crack nucleation and growth for any kind of external loading. Using a metal matrix composite and a coated material as examples [25,26], a complex nonhomogeneous stress–strain state at the micro (meso) scale level is shown to give rise to local microvolumes that increase even under external compression.

The examined finite-difference model for the welded steel (Fig. 4(a)) hardly meets the requirement of a high mesh resolution imposed by cracking calculations. For this reason we did not perform direct simulations of crack evolution but analysed prerequisites for crack nucleation in tension or compression.

According to the fracture criterion used in [25,26], a local region of the material will fail if its relative volume grows and the local equivalent stress $\sigma_{eq}$ reaches the strength limit. The dotted curves with solid and open boxes in Fig. 8 show the volume content of local regions undergoing positive triaxial strain ($\varepsilon_{kk} > 0$) under external tension or compression, respectively. It is not surprising that most of the material subjected to tension demonstrates a volume increase (solid boxes, Fig. 8). Since the highest equivalent stresses develop on the surface, crack nucleation in tension is expected to occur there.

A different pattern is observed under external compression (Fig. 9). The positive volume strain regions are absent in the elastic loading stage, but they are seen awake of the LB front and disappear behind it (open boxes, Fig. 8). The LB front ceases to propagate, the regions of $\varepsilon_{kk} > 0$ localize along the interface between the base metal and the HAZ in the bulk of the material rather than on the surface. The volume content of the regions undergoing triaxial tension increases nonlinearly in the strain-hardening stage. On further loading microcracks are expected to nucleate in these regions as soon as the local equivalent stress reaches the strength limit. Thus, in contrast to tension, compressive cracks are expected to appear not on the surface but in the bulk of the material near the interface between the HAZ and the base metal. Since local equivalent stresses in the bulk of the material are lower than those found on the surface, crack nucleation in compression is expected to occur in a later stage in the compressive deformation process than in tension. This conclusion is consistent with experimental evidence [5].

### 5. Summary

Mesoscale deformation phenomena in a welded low-carbon steel specimen have been simulated numerically. A three-dimensional microstructure-based model was developed to reproduce a gradual change in the grain size in the heat-affected zone-to-base metal transition region. Constitutive relations of polycrystalline grains accounted for the Hall–Petch effect, strain-hardening behavior and difference between the elastic moduli of grains. A double-limit yield criterion was used to describe Lüders band propagation in the base metal.
Stress and strain evolution at the mesoscale level was analysed and the following conclusions were drawn:

(i) In the examined welded steel, there exist several kinds of interfaces responsible for different degrees of stress concentration, i.e., the grain boundaries, the heat-affected zone-base metal and heat-affected zone-fusion zone interfaces, a Lüders front as an interface between the elastically and the plastically strained material, and the specimen free surface. The latter one generates the highest stresses at the mesoscale. A combined effect of the interfaces provides the highest stress level on the surface near the imaginary interfaces between the heat-affected zone and the base metal and between the heat-affected zone and the fusion zone.

(ii) Early plastic strains develop in the surface grains of the base metal near the specimen end where the load is applied. Accordingly, a yield tooth is formed in the macroscopic stress–strain curve. Plastic deformation evident as the Lüders front propagates along the specimen. The effect is associated with the horizontal portion of the macroscopic curve. The Lüders front ceases to propagate as it reaches the HAZ boundary and further plastic flow localizes in the base metal. From this point on the strain-hardening stage in the macroscopic stress–strain curve commences.

(iii) Crack nucleation is expected to occur on the surface under tensile loading and in the bulk under external compression near the interface between the heat-affected zone and the base metal.

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