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Hybrid Approach to Describe and Understand the Influence of Inclusions on the Transition Behavior of X65 Pipeline Steel

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Abstract

Within the last decade, the European steel industry has made impressive progress in providing pipeline steels with excellent mechanical properties. Continuous improvement of cleanliness and tailored thermomechanical treatments lead to damage tolerant microstructures. These steels offer high strength as well as impressive impact toughness properties with upper shelf values of more than 250 J. However, some of these steels show special fracture phenomena such as inverse fracture, separations and a contracted transition area. The last of the three mentioned phenomena is characterized by the simultaneous occurrence of upper and lower shelf values at the same testing temperature during Charpy impact test. This unusual toughness behavior subsequently leads to difficulties in the component safety assessment and needs to be fundamentally understood. In this study, a combined experimental and numerical method is developed to investigate the microstructural reasons of such a fracture behavior. The methodology is demonstrated on a X65 pipeline steel that features a bainitic microstructure and shows a very narrow transition behavior. Following the characterization of the mechanical property profiles of the pipeline steel by different experiments on the meso-scale (e.g. Charpy impact test), the underlying fracture mechanisms were studied. It can be noted that inclusions are identified to be crack initiating for both ductile and brittle fracture behavior. In order to be able to understand the influence of the shape and location of the different inclusions on the fracture behavior, representative volume element (RVE) simulations were carried out. Through the integration of a crystal plasticity (CP) model, the material behavior is simulated at microstructure level and inclusion-related stress concentrations can be discussed. In the future, this approach can be applied to better understand microstructure-related phenomena as well as to couple scale-bridging simulation methods for a material-oriented component design.

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1. Introduction

With the primary aim of avoiding natural catastrophes and supplying the world population with fossil fuels, steel and pipeline manufacturers have achieved great progress in the development of durable and highly performing materials over the last decades. Both process-technological and alloying-related further enhancements allowed not only a significant increase in the strength level (e.g. X120), but also a considerable improvement in the toughness behavior of modern pipeline steels compared to previous grades, so that nowadays upper shelf values of above 250 J can be achieved. This advancement has enabled resources to be saved and thus lightweight construction potential to be exploited without compromising component safety (Rosado et. al. 2013) (Hwang et. al. 2005) (Lenz et. al. 2018).

However, in addition to the positive development trends, modern pipeline steels exhibit fracture phenomena that have not yet been fully investigated. These phenomena are for instance the inverse fracture behavior and the occurrence of separations during Charpy impact test and battelle drop-weight tear test (BDWTT). Several research activities are currently aiming to determine potential root-cause analyses, evaluation methods, and effects on component behavior. Another phenomenon, which is also present in modern materials, but receives less attention in literature, is the contracted or overlapping transition behavior that can be seen in Charpy impact test. A characteristic feature is the simultaneous occurrence of upper and lower shelf behavior at identical test temperatures. Currently it is uncertain to what extent this material behavior influences the component performance of pipelines. In order to characterize and describe this influence, a fundamental understanding of the underlying mechanisms of the occurring phenomenon on the one hand and a method to determine the influence on the component performance on the other hand are required (Hwang 2004) (Sha 2013).

This paper presents a hypothesis on the occurrence of the contracted transition behavior of an X65 pipeline steel, which shows the described phenomena. A hybrid methodology is developed on the microscopic scale to gain a deeper understanding of the releasing mechanisms.

2. Material characterization

In this study an X65 Q+T (quenched and tempered) pipeline steel with a material thickness of 19 mm is investigated. The chemical composition of the material can be found in table 1.

Table 1. Chemical composition of X65 pipeline steel, in wt.-%.

C	Si	Mn	P	S	Cr	Mo	Ni	Ti	V	Nb	N	B
0.044	0.35	1.52	0.01	0.002	0.05	0.009	0.231	0.015	0.002	0.037	0.01	0.001

As it can be seen in Figure 1, the steel features a bainitic microstructure with minimal phase fraction of martensite and retained austenite that represents less than 1 % of the total microstructure. Light-optical findings show that both, calcium sulfides (CaS) and titanium nitrides (TiN) are present in the microstructure. Under quasi-static tensile test conditions at room temperature the material shows a continuous yielding, which starts at 593 MPa. The tensile strength lies at 742 MPa, while a fracture elongation of 19.6 % was measured using a round tensile test specimen B8x40. The mechanical properties are summed up in table 2.

Table 2. Mechanical properties of X65 pipeline steel under quasi-static test conditions at room temperature.

Yield strength	Ultimate tensile strength	Uniform elongation	Total elongation
[MPa]	[MPa]	[%]	[%]
593	743	6.3	19.6

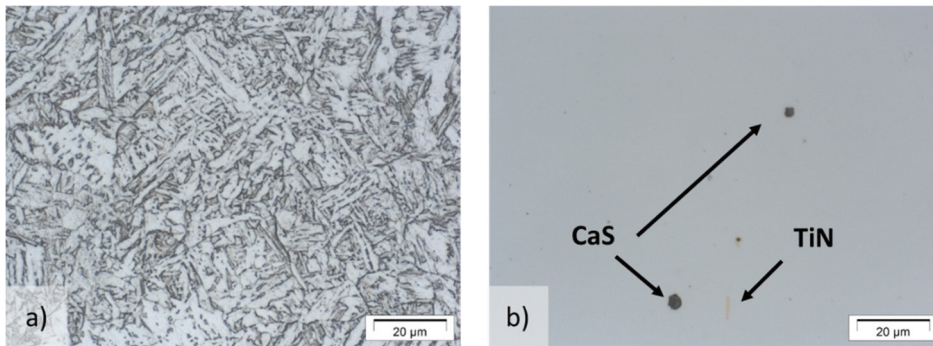


Fig. 1. Bainitic microstructure of X65 pipeline steel (a); CaS and TiN in the microstructure of X65 pipeline steel (b).

The transition curve determined from the Charpy impact test shows a contracted transition behavior around 0 °C, where upper and lower shelf values occur at the same testing temperature. An average energy level of 43 J is reached in the cleavage fracture area between -10 °C and -60 °C. On the other hand, upper shelf values of more than 350 J were reached. The temperature-dependent impact energy behavior of the X65 steel can be seen in figure 2.

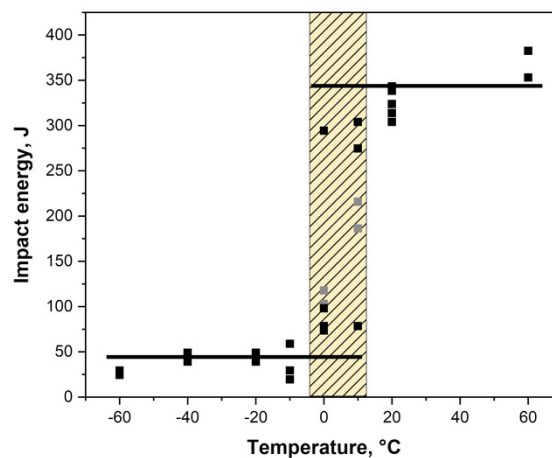


Fig. 2. Temperature-dependent impact energy behavior of the X65 steel with a contracted transition region

3. Hypothesis and methodology development

To assess the uncertainties in the component design resulting from the material behavior that can be seen in figure 2, a fundamental understanding of the reasons for the occurrence of a contracted transition behavior is required. In addition to the influencing variables to be considered, such as temperature, strain rate or stress state dependence, a decisive role is attributed to the microstructural investigation of underlying mechanisms. For this reason, the fracture behavior and the origin of failure was first investigated using scanning electron microscopy (SEM) examinations. The focus was placed on the fracture behavior of Charpy impact test specimens at a test temperature of 0 °C, as both upper shelf and lower shelf behavior occurs in this area. Based on these fracture surface investigations it could be shown that the initiation of cleavage and ductile fracture is located at inclusions. The inclusions are mainly TiN and CaS, but oxides have also been detected. Figure 3 shows the fracture surfaces of specimens tested at the same temperature with

different fracture behavior. From the findings it can be concluded that inclusions are the crack initiating microstructural features.

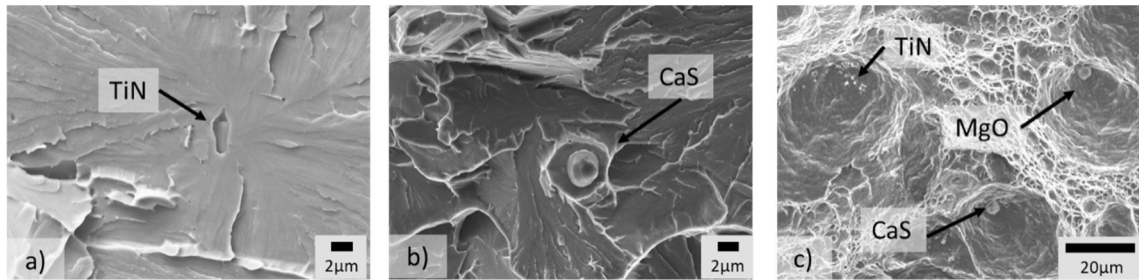


Fig. 3. Cleavage (a, b) and ductile (c) fracture and damage initiation points of Charpy impact test specimens at 0°C.

However, it is not clear at this stage why certain void formation respectively microcracks result in a cleavage fracture event, while others lead to a ductile fracture behavior. This mechanism needs to be understood fundamentally, in order to be able to draw conclusions about the occurrence of a contracted transition behavior and subsequently identify possible solutions to prevent this phenomenon. The authors therefore proposed the hypothesis that an unfavorable position of the inclusion within the microstructure leads to the critical cleavage fracture event due to high local stresses and strains, while a favorable positioning of the respective inclusion will result in a ductile fracture. To validate this hypothesis, critical positions of the inclusions, e.g. at grain boundaries or the orientation of the inclusion to the direction of loading, need to be identified. Furthermore, it is necessary to reconstruct the crack origin depending on the local microstructure. Since a purely experimental validation of this hypothesis is resource-consuming, a hybrid, scale-bridging method is presented. Based on experimentally determined statistical data such as inclusion and grain size distributions, representative volume elements (RVE) are constructed. In addition to the geometric representation of the microstructure, a mechanical, grain orientation-dependent description of the material behavior is required. The RVE is therefore coupled with a crystal plasticity (CP) model that needs to be calibrated by nanoindentation tests. With these microstructure models inclusions can be positioned as desired and an infrastructure for virtual experiments is set up. By varying the size, orientation and location of the respective inclusion, local stress concentrations can be determined and thus critical positions or features of inclusions will be identified from the simulations. This will allow the hypothesis to be validated in a resource-saving way. In the future, this micromodel infrastructure provides the opportunity to apply scale-bridging methods by deriving fracture related parameters from microscopic simulations for the simulation of macroscopic Charpy impact test.

4. Setup of a microstructure-based simulation environment

RVE are created based on statistical data from electron backscatter diffraction (EBSD) images. For this purpose, the grain size distribution is fitted using a log-normal function and processed by a random sequential algorithm (RSA) and a Voronoi tessellation for further data handling in the FEM software Abaqus. Following the meshing of the RVE in Abaqus, periodic boundary conditions are applied to the RVE. A detailed description of the RVE construction can be found in Gillner and Münstermann, 2017. The material model used in this method development is a crystal plasticity (CP) model, which is based on equation 1-3 (Roters et. al., 2010).

$$\dot{\gamma}^{\alpha} = \dot{\gamma}_0 \left| \frac{\tau^{\alpha}}{\tau_c^{\alpha}} \right|^a \text{sgn}(\tau^{\alpha}) \quad (1)$$

$$\tau_c^{\alpha} = \tau_0 + q^{\alpha\beta} \left[h_0 \left(1 - \frac{\tau_c^{\beta}}{\tau_s} \right)^a \right] |\Delta\gamma^{\beta}| \quad (2)$$

$$\tau^\alpha = \sigma[m^\alpha \otimes n^\alpha] \quad (3)$$

These equations describe the slip rate (eq. 1), the resolved shear stress (eq. 2), and the critical resolved shear stress (eq. 3). To calibrate the model, nanoindentation investigations are performed on four grains of different orientation. The grain orientation dependent force penetration depth diagrams can be used to determine the CP parameters. For this purpose, the nanoindentation tests are modeled in the FEM software Abaqus and the numerical curve is iteratively approximated to the real material behavior by varying the corresponding parameters τ_0 , τ_c^α , h_0 , and α . The material depended CP parameters for the X65 pipeline steel are shown in table 3.

Table 3. Crystal plasticity (CP) parameters for X65 pipeline steel.

τ_0	τ_c^α	h_0	α
MPa	MPa	MPa	-
100	1500	1500	1.5

Once the RVE (figure 4a) has been set up and coupled with the material model, virtual experiments can be performed. For this purpose, TiN with different edge lengths (1mm, 2.5mm and 7.5mm) and variable orientation (0° and 45°) are embedded into the digital microstructure model. The material properties of TiN are assumed to be fully elastic with a young's modulus of 600 GPa and a poisson's ratio of $\mu = 0.295$ (Perry 1990) (Zhang 2001). The different test cases can be seen in figure 4b. Additionally, the approach of embedding a void that has a similar geometry to the TiN into the microstructure is followed, thus extending simulations with TiN-like voids, so called cut-outs, to the virtual test matrix. This approach is based on the assumption that even small deformations lead to decohesion between the inclusion and the microstructure matrix.

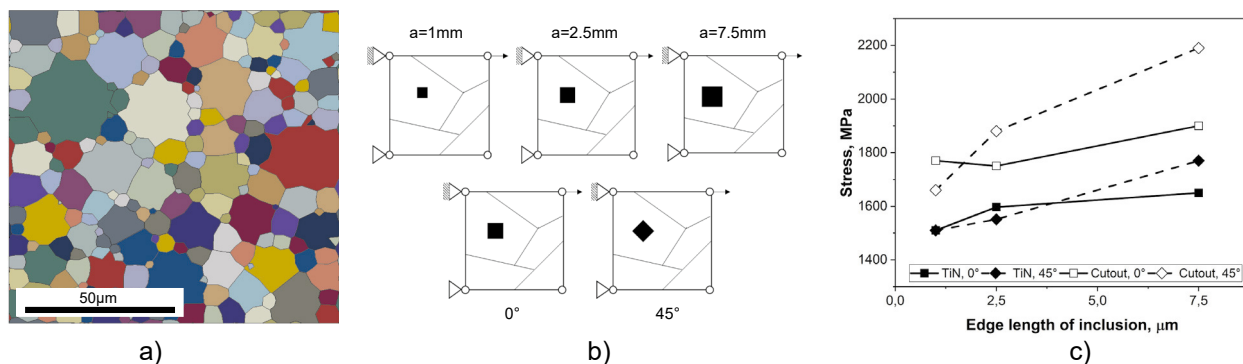


Fig. 4. Representative volume element (RVE) of X65 pipeline steel (a), virtual test scenarios (b) and local stress concentration at inclusion depending on the position, mechanical description and size of TiN (c).

Figure 4c shows the maximum local stresses in one element at the TiN and the cut-outs depending on the edge length. Filled symbols (black) display the TiN, while symbols without filling (white) represent the cut-outs. From the results it can be seen that the maximum local stress at the inclusion increases with higher edge length. A growth in edge length results in an increase in the local accumulation of dislocations, thus causing an elevated stress at the inclusions. Furthermore, it can be noted that a tilting of the inclusion with higher edge lengths by 45° also leads to an increase of the local stress concentration, which can be explained by the notch effect in deformation direction. Simulations which take into account the properties of a TiN inclusion generally show a local stress level that is about 150-500 MPa lower compared to the numerical investigations with cut-out.

5. Conclusion and Outlook

In this study a fully bainitic X65 pipeline steel was studied. The focus was placed on a hybrid methodology development for the microstructural description of the contracted transition behavior. The main conclusions are:

- Experimental results show a contracted transition behavior at a temperature of 0 °C. Around this temperature upper and lower shelf values occur at the same testing temperature, which leads to challenges in the component design.
- TiN and CaS inclusion were identified as crack initiation points for cleavage and ductile fracture events.
- A hybrid methodology was presented to identify the microstructural causes for the observed contracted transition behavior in X65 pipeline steel. Representative volume elements (RVE) and crystal plasticity (CP) model are used to perform virtual experiments with different positions and sizes of TiN inclusions.
- The microstructure model shows a strong dependency of the local stress concentration on the edge length and the position of the TiN inclusion, which indicates that the meso-scale behavior, e.g. toughness behavior, can be attributed the position and size of the inclusion. To fully prove the hypothesis further numerical investigations are needed.

In the future further virtual experiments will be carried out to gain a deeper understanding of critical position of TiN and CaS inclusions. Besides local stress concentrations, the strain concentration at inclusion will be analyzed in upcoming studies. In addition to the mechanism study, the presented microstructure simulation infrastructure can be used for an alternative parameter calibration of the macroscopic damage model. In order to evaluate the macroscopic material behavior and the component performance, virtual experiments on the microscopic scale will be performed under different stress states in future work to couple the mechanical response of the microscopic model with a macroscopic damage model. The toughness behavior of the X65 pipeline steel can then be predicted using microstructure-dependent fracture locus.

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