Abstract

The present thesis explores the micromechanics of cleavage (or, brittle) fracture in steel across different length scales, encompassing the microstructural, crystallographic, and atomic levels. The aim is to comprehend the fundamental pathways for improving the low temperature cleavage fracture resistance of steel. Besides, it is the ductile to brittle transition (DBT) phenomenon, which is primarily responsible for promoting cleavage fracture at low temperatures in steel. While the microstructure plays an important role in altering the shape of the DBT curve, the atomistic origin of the DBT phenomenon lies in the BCC crystal structure of Fe. Therefore, the present work investigates both the microstructural as well as atomistic aspects of cleavage fracture in steel, employing both experimental and simulation approaches.

To study the effect of microstructure on the cleavage cracking behavior, three different steels were selected in this work, namely ferritic, pearlitic, and martensitic steels. Suitable heat treatment schedules were adopted to get the desired microstructures in each of those steels. All the heat-treated steels were subsequently subjected to Charpy impact test, which is a standard industrial practice to determine the DBT curves of steels. Depending on the DBT temperatures (DBTT) of the present steels, the impact test was conducted at sufficiently low temperatures to ensure complete brittle failure., e.g., the test temperature was -120 °C for ferritic steel, room temperature (24 °C) for pearlitic and -196 °C for martensitic steels. As a note, the presence of continuous and closely-spaced brittle cementite lamellae in pearlite microstructure makes the steel brittle even at room temperature. Subsequent analyses of the cleavage crack path were made on the transverse sections of the broken Charpy specimens using SEM and EBSD. The most preferred crystallographic cleavage plane in all the steel microstructures is {100}. However, occasional cracking along {110} plane is also feasible, specifically when the {100} planes of a given grain possess high twist and/or tilt misorientation angles with the preceding crack plane. The contribution of {110} cracking is maximum in pearlite, minimum in ferrite and intermediate in martensite microstructures. The preference of {110} cracking in the pearlitic steel has been correlated with the restricted crack tip dislocation emissions due to limited slip transferability across the ferrite/cementite interfaces, which thereby facilitates cleavage cracking along the lower energy {110} planes as compared to {100}. In addition, the effect of pearlite

lamellae orientation on fostering the interplay between cleavage cracking and ferrite/cementite interface cracking is also extensively discussed using an appropriate mathematical model simulation.

Besides, cleavage cracking along {100} planes is often associated with the formation of numerous “tongue” like features that are intermittently aligned parallel to a common <110> crack front. To illuminate the origin of such intermittent tongues, molecular dynamics (MD) fracture simulation was performed on a pure Fe single crystal, considering a (001) edge crack with a large [110] crack front. It was found that the development of intermittent tongues mainly originates from the intermittent nucleation of symmetric {112}<111> type twins across the entire crack front. Based on the simulation results and experimental observations, a step-by-step mechanism is proposed that potentially explains the formation of intermittent tongues when a sufficiently large <110> straight crack front propagates along a {100} cleavage crack plane.

Using the classical Rice model of crack blunting by dislocation emission, a theoretical model has been proposed to study the effect of crystallographic orientation of ferrite grains on the intrinsic crack resistance, which represents the inherent resistance offered by the BCC Fe lattice against cleavage crack propagation. In other words, the proposed model predicts suitable grain orientations (texture components) in a polycrystalline steel that can potentially improve its low temperature cleavage fracture resistance. Besides, the beneficial effect of alloying additions on further improvement in the intrinsic crack resistance of steel is also discussed, pertaining to the role of unstable stacking fault energy.

Since the low temperature fracture resistance of steel is mainly deteriorated by the DBT phenomenon, the present thesis also delves into the atomistic origin of DBT phenomenon, which lies in the interplay between the flow stress and fracture stress sensitivity towards temperature variation. The restricted motion of screw dislocation in BCC Fe lattice results in a high Peierls stress at 0 K and a pronounced temperature sensitivity of flow stress, primarily responsible for encouraging the DBT phenomenon. In this respect, addition of suitable alloying elements, like Ni, is believed to improve the low temperature fracture toughness by reducing the temperature sensitivity of flow stress. Using molecular statics simulation, the present work predicts that the local distribution of Ni atoms around the screw dislocation greatly influences the Peierls stress of BCC Fe, governed by the local distortion of the dislocation core structure by the solute atoms.

Considering a random solute distribution in Fe-Ni alloys, the MD simulation results show that increasing the Ni concentration helps in reducing the temperature sensitivity of flow stress by inducing solid solution softening effect at low temperature regime. The rationale behind the softening action of Ni is discussed in terms of the distortion in dislocation core structure and reduction in USFE of Fe.

Finally, the role of Ni in tailoring the DBT curve of BCC Fe was investigated by employing MD fracture simulation of different binary Fe-Ni alloys. The DBT curves are subsequently correlated with the temperature sensitivity of fracture stress, estimated using the concept of critical strain energy release rate (G_{IC}). The role of Ni in reducing the fracture stress sensitivity is responsible for decreasing the DBTT as well as the slope of the DBT region. The underlying mechanism is discussed in terms of the crack blunting effect of Ni which effectively increases the G_{IC} and hence the fracture stress, particularly at the low temperature regimes. Besides, the present work also tackles the inherent strain rate issue of MD simulation, in predicting higher DBTT values, by using an appropriate strain rate sensitivity factor to rescale the simulated DBTT values down to the experimental ones, resulting in a good match between the simulated and experimental DBTT.

Thus, the present thesis brings together the microstructural, crystallographic, and atomistic aspects of cleavage fracture that offer potential avenues for tackling the catastrophic brittle failure of steel at low temperatures.

Keywords: Steel; Microstructure; Crystallography; Cleavage fracture; Ductile to brittle transition; Tongue; Screw dislocation; Dislocation emission; Intrinsic crack resistance; Flow stress; Fracture stress; Molecular dynamics simulations