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The atomic-scale origins of liquid metal embrittlement in the Fe-Zn system

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Extended Abstract

Abstract

Liquid metal embrittlement (LME) refers to the reduction in ductility and toughness of a solid metal when in contact with liquid metals. This kind of material property degeneration poses a serious challenge for several industrial sectors, including the automotive industry. There, the embrittlement of advanced high-strength steels by their liquified Zn-coating during welding is of major concern. This makes Fe in contact with liquid Zn a highly relevant example of an LME-susceptible metal couple. To aid the elucidation of the atomic-scale origins of LME, we established an atomistic simulation framework to assess fracture processes (brittle and ductile) along general grain and phase boundaries as well as in generally oriented single crystals. This framework takes the form of a K-test molecular dynamics (MD) setup for interfacial cracks. The simulation domain, i.e. the near-crack tip region, is constructed using the Stroh formalism — an approach from linear elasticity theory for modelling cracks along arbitrarily oriented dissimilar anisotropic interfaces. The second crucial ingredient for reliable predictions of material properties, using MD approaches, is the choice of a suitable interatomic potential (IAP) to describe the interactions between the system's atoms. For our studies, we developed a new machine-learning (ML) IAP for the Fe-Zn system based on the atomic cluster expansion (ACE) method, as the resulting potentials offer a superior balance of accuracy and evaluation speed. With the developed ML IAP, it is possible, for the first time, to reproduce general and fracture-related properties of the Fe-Zn system with sufficient accuracy to study complex

fracture phenomena such as LME. The last key component for physically meaningful assessments of LME is a realistic Zn distribution in the vicinity of the crack tip and along grain boundaries (GBs). Such a distribution arises from the diffusion of Zn from the material's surface along GBs and into the bulk during, e.g. welding. From an atomistic modelling perspective, such diffusive timescales in the order of milliseconds to seconds are inaccessible due to the short time step size (femtoseconds) in MD simulations. For this reason, we devised a multi-time-scale framework for obtaining the required initial conditions: The atomistic simulation domain is mapped onto a finite element discretisation, in which a stress-assisted GB diffusion equation is solved for the timespan and temperature under consideration. The relevant model parameters are thereby either obtained from MD (e.g., diffusivity) using the developed ML IAP or from analytical theory (e.g., stress fields), making the outlined approach parameter-free. With the established and fully validated K-test framework, we are able to obtain new insights into the atomistic origins and effects of LME at the atomic scale. Our research thereby focuses on quantifying the degradation of Fe's fracture toughness as a function of Zn content and distribution. However, it is well known that LME strongly depends on temperature, strain rate effects, the character of the considered grain boundaries and the formation and fracture behaviour of Fe-Zn intermetallics. Hence, we consider all of these influencing factors in our fracture studies to aid the elucidation of LME through novel atomistic insights.

Keywords:

liquid metal embrittlement K-test atomistic fracture simulations machine learning interatomic potential molecular statics grain boundaries