Project Network 3 “Data-Integrated Model Reduction for Particles and Continua”

PN 3-10: “Simulations of hydrogen embrittlement in Ni-based super alloys”

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State of the Art and Preliminary Work

Ni-based superalloys consist of a distinctive microstructure designed to provide good high temperature creep behavior. A main strengthening mechanism in these alloys relates to the γ/γ' interfaces, with dislocations primarily moving through the Ni fcc based channels and with the Ni_3Al γ' precipitates acting as dislocation blockers. Depending on the exact composition and ageing state, other phases such as the γ'' and δ phase can also be present. Ni-based superalloys exhibit a pronounced embrittlement at intermediate temperatures (600 °C to 700 °C) [L1] which is not understood so far, although several mechanisms have been proposed such as intergranular precipitates, grain boundary shearing, gas phase embrittlement, glide plane decohesion, dynamic strain ageing and grain boundary segregation.

Current experimental investigations support several of the aforementioned mechanisms. The work of Chung [L2] shows that with increasing temperature the deformation mechanism changes from γ' shearing to bypassing of these precipitates and identifies this as glide plane decohesion. This observation could be also caused by a change in the APB energy of dislocations in the γ' phase due to thermal effects, the determination of which is one of our main goals. Regarding gas phase embrittlement, Han [L3] found that hydrogen leads to cracking at grain boundaries due to the formation and coalescence of nano-voids at hydrogen saturated dislocations at the grain boundaries. The works of Obasi [L4] and Zhang [L5] show that the presence of δ and γ'' precipitates leads to grain boundary decohesion in the presence of hydrogen.

MD simulations [L6] have shown that hydrogen leads to a weakening of the γ/γ' interface due to the interaction of hydrogen with the regular misfit dislocation network, hinting towards hydrogen-enhanced decohesion (HEDE). Another finding of one of the project’s PIs [L7] is that hydrogen at dislocations can result in the formation of nano-hydrides which support the embrittlement via dynamic strain ageing. Most of the existing MD investigations use radial symmetric embedded atom method (EAM) potentials, due to which diffusion processes that rely on accurate orientation dependent energy barriers are oftentimes not described well enough. One remedy is to use bond order potentials such as Tersoff or ReaxFF which encompass a more complex description of the angular dependence of interatomic interactions. In this project, we aim to use the ML-based MTPs [L8, L9] in order to capture the complex diffusion behavior from the ab initio data implicitly.

Project Goals and Work Schedule

The project aims at the development of an accurate interatomic potential for the Ni-Al-H material system. Main challenges therein are the interactions with the hydrogen atoms which, due to their quantum nature as the lightest element, will have substantial angular dependent contributions to

the overall energy, which are lacking in classical potentials such as EAM. In order to parametrize the potential, a ML-based approach will be employed which will learn from results obtained by DFT. The accurate interatomic potential will efficiently provide the needed data for determining the Gibbs free energy of the γ' APB via thermodynamic integration. At the same time, the potential will allow for direct simulation of hydrogen diffusion in γ/γ' microstructures deemed too large for classical ab-initio approaches enabling the identification of hydrogen binding sites and storage capacities as well as studying the effect of hydrogen on grain boundary (GB) decohesion.

In order to parametrize the interaction of Ni, Al and H, a large amount of first principles calculations will be conducted which will provide the input data for the ML-based MTP model. This model is then trained on the input data with the aim of deriving a precise but fast approximation suitable for use in large scale MD calculations on hydrogen diffusion that will clarify the role of hydrogen in gas phase embrittlement by quantifying preferential H-sites and change in work of separation. Additionally the MTPs will also be used for thermodynamic integration in order to determine the temperature dependent Gibbs free energy of the APB found in γ' precipitates, which will provide insight into the role of dislocations in γ/γ' microstructures in intermediate temperature embrittlement. The detailed working program consists of the following work packages:

WP 1 (9 months): Ab initio calculations of structures in the Ni-Al-H material system
WP 2 (12 months): Optimization of moment tensor interatomic potentials for the Ni-Al-H system
WP 3 (12 months): Calculation of the temperature-dependent antiphase boundary energy in Ni_3Al
WP 4 (9 months): Large-scale molecular dynamics simulations of H diffusion in Ni-Al alloys

Literature

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