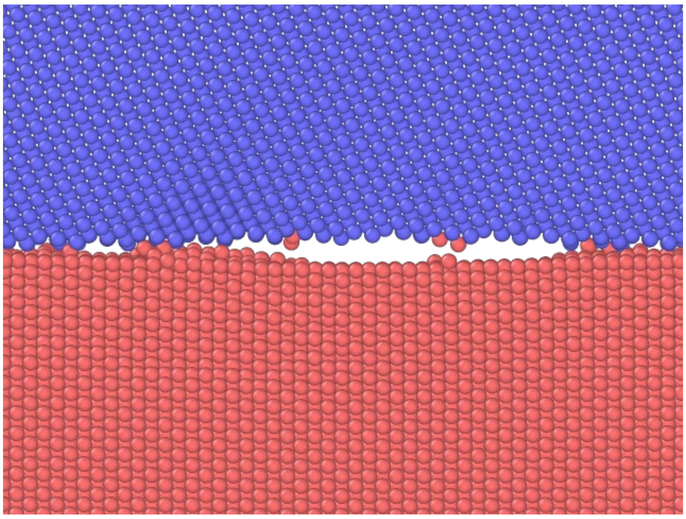
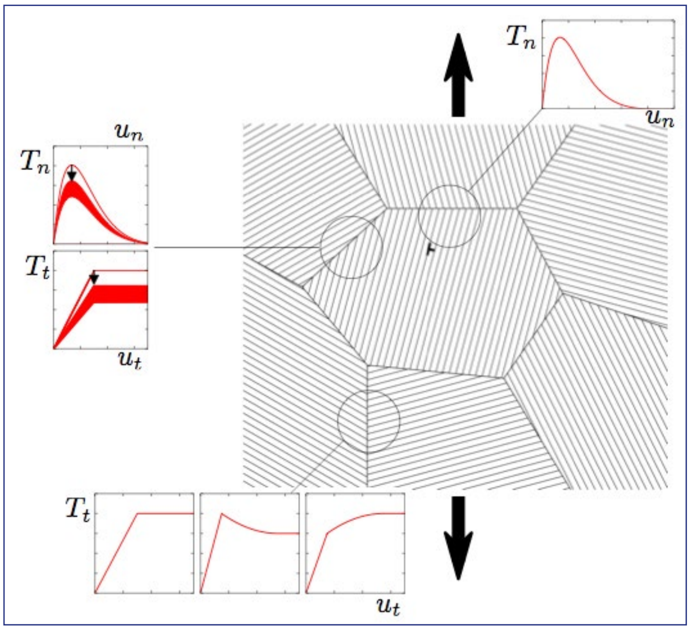
‘Nano-scale failure in steel: Interface decohesion at iron/precipitate interfaces’

Multiphase alloys such as advanced high strength steels can show unexpected failure due to dislocations piling up at internal boundaries between the soft iron matrix and the hard precipitates. The stress concentrations caused by the dislocation pile-ups might trigger interface decohesion followed by the formation of voids and, eventually, macroscopic cracks. To prevent such material failure, accurately predictive material models are needed.

Dr.ir. Astrid Elzas studied together with prof.dr. Barend Thijsse crack nucleation and interface decohesion on the nanoscale with large-scale molecular dynamics simulations, to understand which conditions lead to interface decohesion. Systematically varying different physical parameters allowed clear observation of the important physical effects in a controlled manner. Not only where the studied interfaces and the numbers of dislocations piling-up at the interfaces varied, also different loading modes where considered. Apart from pure shear and pure tensile loading, in this study also mixed loading, i.e. a tensile force under an angle with the interface, was considered. It is found that the interface structure, which changes during response to loading, is the key factor determining the material response.



Molecular dynamics simulation of interface decohesion at an interface between the soft iron matrix (red) and a hard precipitate (blue) of steel



Schematic representation of various interfaces subjected to different loading modes, due to their orientation. Various relations between tractions and separations are found for the different interfaces and different loading modes

Apart from the deeper and systematic understanding of interface decohesion resulting from this study, also interface/material-specific traction-separation relationships are developed which can be applied in larger scale material models to improve the accuracy of this models with respect to the description of interface behaviour and with that lead to a better prediction of material failure.

On 10 January 2019 Astrid Elzas obtained her Doctorate cum laude for her thesis ‘Nano-scale failure in steel’ at Delft University of Technology.

The thesis can be found at:
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