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An interface model to account for damage and plasticity at grain boundaries

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Grain boundary (GB) characteristics play a major role in the understanding and prediction of polycrystalline behavior [1]. GB roles become more important when it comes to nanocrystalline metals and ceramics. To gain a deeper insight into the behavior of the grain boundary, molecular dynamics (MD) simulations are utilized. The Mode I, mode II and mixed mode loading behavior is investigated using different MD simulations. By adding the unloading path to the MD simulations it was possible to differentiate between different active mechanisms at the GB. An interface model is introduced based on our understanding from the atomistic simulation of the grain boundaries. When it comes to the grain boundary (GB) behavior, the current model is able to capture the competition between the intergranular fracture and the grain boundary sliding. The interface model is thermodynamically consistent and is able to capture the complex behavior of the GB under different loading conditions.

1 Idea behind traction density

A new approach is introduced in which instead of defining relation for tractions in terms of jumps at the interface, traction is going to be computed based on a new quantity called traction density. In this work, the traction vector $\boldsymbol{t}$ is obtained by integrating the values of the traction density vector $\boldsymbol{T}$. In the Fig. 1, an interface in the current configuration is shown. The vector $\boldsymbol{x}_i^+$ represents the current position of the point i on Γ^+. For each point $\boldsymbol{x}^-$, the local gap vector $\boldsymbol{G}_i(\boldsymbol{x}^-)$ is defined, which represents the vector from an arbitrary point on Γ^- to the point i. The distribution of the traction density vector is represented by $\boldsymbol{T}_i(\boldsymbol{x}^-)$.

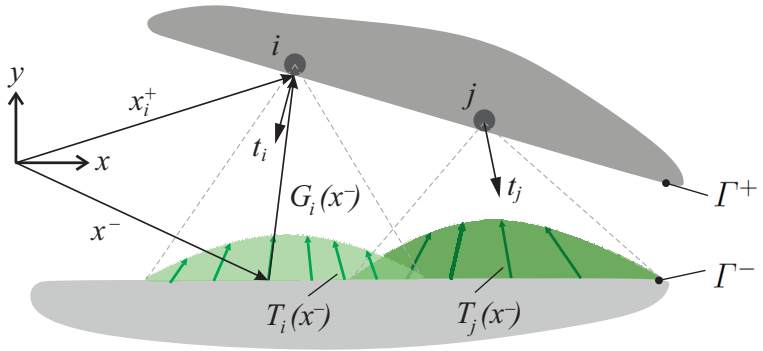

Fig. 1: The connection between traction and traction density vector in the deformed configuration.

In general, $\boldsymbol{T}$ is a function of the local gap between the two arbitrary points and other internal variables, i.e. $\boldsymbol{T}_i = \boldsymbol{T}_i(\boldsymbol{G}, \underline{\boldsymbol{v}})$. As in the current work the focus is on the behavior of the GB, the only internal variable will be the scalar damage variable D. Finally, as explained before, the traction vector is computed by summing up the traction density

$$\boldsymbol{t}_i = \int_{\Gamma^-} \boldsymbol{T}_i \, d\Gamma^- \tag{1}$$

It should be pointed out that the area (segment) on Γ^- which has an influence on Γ^+, depends on the nature of the problem. For each arbitrary point i shown in Fig. 1, the dashed lines represent the area on the lower interface Γ^- which influences the point i. In the current work, it is assumed that the two surfaces attract each other by means of atomistic forces. Therefore, the traction density vanishes eventually as the distance between the interfaces increases.

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2 Formulation of traction density for the grain boundary

On the right side of Fig. 2, the traction vector $\boldsymbol{t}$ and its components in normal and shear direction are shown. The traction vector, in general, is of anisotropic nature [1] for which utilizing classical interface modeling is problematic and one needs alternative extensions [2]. Here, by using the idea of traction density we try to overcome this problem. The traction density vector $\boldsymbol{T}$ is defined as a quantity which describes the interaction between the two interfaces and it is assumed to be co-linear to the local gap vector $\boldsymbol{G}$. Moreover, the blocks of atoms are large enough so that one should consider structural features such as damage.

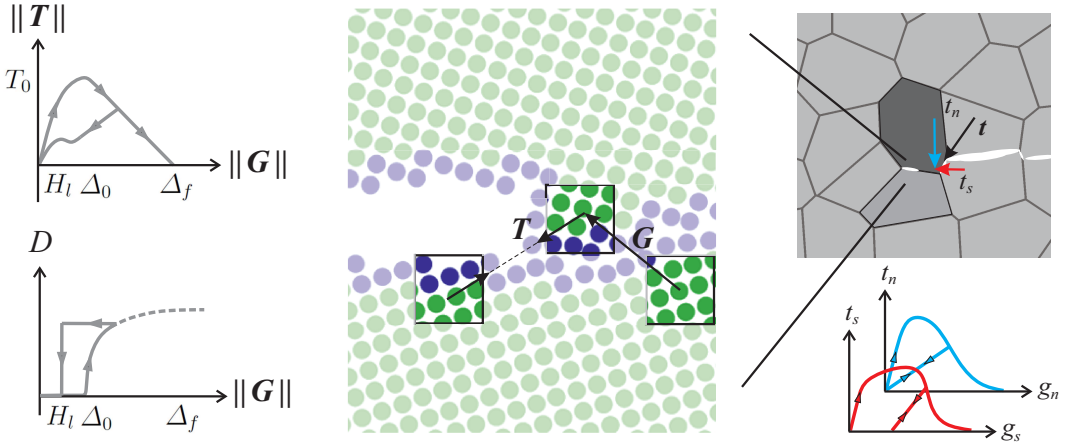

Fig. 2: Formulation of traction density at the grain boundary.

The relation for the traction density is $\boldsymbol{T} = (1 - D)\,\dfrac{T_0}{\Delta_0}\,\boldsymbol{G}$. where Δ_0 is the distance at which the maximum traction density is reached, Δ_f is the distance at which the traction density vanishes and H_l is the healing distance parameters.

3 Numerical results and comparison with MD simulations

A comparison is made between the obtained traction-separation relation from the model and the results of the atomistic simulations. For this purpose, aluminum (with $\Sigma 5$ GB) is chosen and the atomistic simulations are performed using LAMMPS (see also [1]). The parameters for the interface model are fitted to the results of the MD simulations. These comparisons are shown in Fig. 3 for mode I and mode II loadings which show a good agreement with MD calculations.

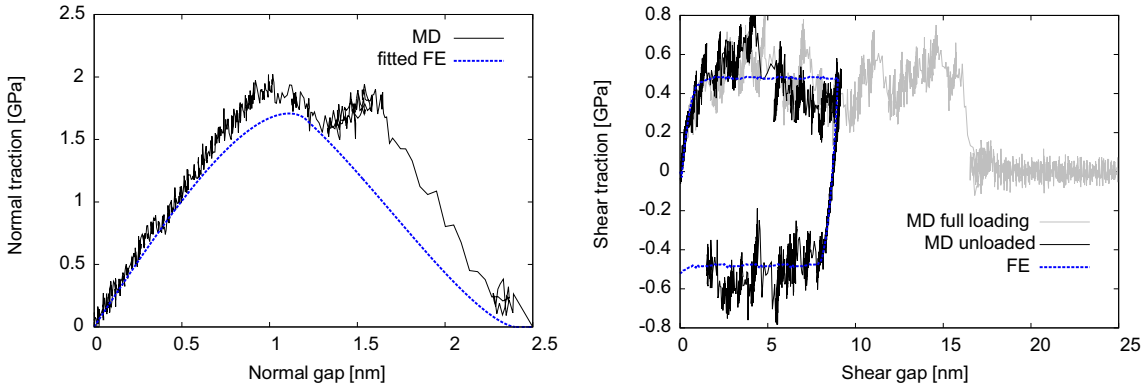

Fig. 3: Comparison of the FE and MD results.

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