Multiscale Metallic Interface Modelling – MuMiM

STW-project in the programme Multi-Scale Simulation Techniques

Participating groups

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Structure and Change in Materials - Joining and Mechanical Behaviour

Vacancies (PhD)

1 PhD vacancy at the University of Groningen
1 PhD vacancy at Delft University of Technology
1 PhD vacancy at Eindhoven University of Technology

1. Summary

Metallic interfaces, such as grain boundaries, phase boundaries and metallization layers, play a dominant role in bulk materials, functional materials and metallic microdevices in defining their strength, reliability and lifetime properties. Nevertheless, the current modelling of metal interfaces is still rather rudimentary, being at best limited to standard anisotropy boundaries and, even more exceptionally, to cohesive zones. The latter models describe debonding but they neglect the critical interaction between plasticity and interfaces. This interaction takes place at the level of individual dislocations that can be accumulated, transmitted, absorbed or nucleated at the interfaces. A better insight and quantification of these mechanisms at interfaces with different characteristics can only be gained through detailed analysis of these processes across the scales: from the atomistic level via the level of discrete dislocations to the continuum interface level — coupled by means of proper scale transitions. This project aims at constructing a generic multi-scale technique for the quantitative description of metallic interfaces, developed on the basis of a complex grain boundary as a carrier problem. The research is organised in 4 interrelated workpackages (WP). A molecular dynamics (MD) model of dislocations interacting with complex large angle grain boundaries will be created within WP1 (PhD vacancy in Delft), and the respective constitutive rules for the discrete dislocation (DD) simulations will be derived using a dedicated coarse graining approach. These DD constitutive rules will be applied in WP2 (PhD vacancy in Groningen) to model the collective behaviour of dislocations being absorbed, stored and nucleated at the interface. The DD boundary value problem will be upscaled towards a continuum interface model within WP3 (PhD vacancy in Eindhoven) using a computational homogenization technique. The computed interface response will be used to obtain explicit constitutive equations for the interface that, in turn, will be transferred to WP4, which concentrates on application of the resulting tools to several problems of industrial interest.

2. Research team

The research team that will perform and exploit the project consists of 3 academic partners from different disciplines and 3 industrial partners from different sectors. The academic partners unify their individual strengths on modeling at 3 distinct length scales, while the mutual co-operation will enable the development of the methodology to the required scale transitions. The industrial partners unify a common interest in the behaviour of metallic interfaces, from different application perspectives. The role of each of the partners and staff members involved is listed below.

3 Scientific project description

3.1 Introduction and objective

Metallic interfaces are a key ingredient in controlling the strength, ductility, reliability and lifetime properties of metal-based structural and functional materials and/or devices. This holds for bulk materials, where many properties are controlled by the behaviour at and through physical boundaries (precipitate hardening, Hall-Petch effect, etc.). However, this is even more so for small metallic components, like those used in MEMS where the mechanical properties are largely dominated by the metallic interfaces present (e.g. grain boundaries and oxide layers). Likewise, solder interconnects are prone to failure along interfaces.

To date, very few models can account for the explicit presence of an interface, other than a boundary between domains with a different anisotropy. At the continuum scale, interfaces are sometimes accounted for, implicitly, in the higher-order boundary conditions (BC) used in gradient-enhanced or strain-gradient crystal plasticity frameworks. The BCs used consider the limiting situations of either impenetrable or completely transparent GBs. The main reason for this simplification is the lack of knowledge of the mechanisms occurring at the underlying scale. A few attempts have been made to address the interaction between dislocations and a grain boundary on a phenomenological basis only [60,70]. Interface elements for the failure of interfaces are usually of the cohesive zone type, motivated or derived from atomistic simulations, e.g. [65-67,69,77], but they do not include the interaction between plasticity and interfaces.

This plasticity–interface interaction takes place at the level of individual dislocations, which can be blocked by, absorbed in, transmitted through or nucleated from interfaces in the case of grain boundaries. While major developments were realized in the past two decades that enable the analysis of the interaction of dislocations with each other, with other obstacles and with free surfaces, till this date discrete dislocation (DD) simulations adopt similar simplifying assumptions for the interactions with interfaces as used at the continuum scale, e.g. [31,32,46,48]. At this moment, the first attempts are being made to incorporate the transmission of dislocations through perfect grain boundaries (tilt or twist boundaries) in the EU-NSF project NANOMESO [http://mse.osu.edu/~andersonp/nanomeso.html]. However, the study of dislocation interactions with more complex interfaces is not addressed yet.

Such studies, inevitably, have to be done at the atomic level, where the real interactions between individual atoms are expected to provide the answers that will help resolve the unknowns at larger scales. Somewhat more complex interfaces can be explicitly modelled and the interaction of dislocations with such interfaces can be studied in a rigorous manner. Literature provides some coarse graining (or homogenization) attempts, where molecular dynamics (MD) level is directly embedded in the continuum mechanics (CM) level [64,72,74,75], for a state-of-the-art review, see [63]. This limits the applicability to very small plastic zones and forbids the extraction of coarse-grained descriptions.

Objective

The objective of this research is to develop a generic multiscale methodology that enables a quantitative study of the role of metallic interfaces up to the level of its integration into a complete numerical model of microstructure or microdevice. The project aims to define generic boundary value problems and solution schemes at each length scale that can be used for metallic interfaces in general. Likewise, scale transitions between the MD (molecular dynamics) level and the DD (discrete dislocation) level, and between the DD and continuum interface level are to be developed in a generic manner, i.e. allowing for applications beyond the particular problem used as a carrier. Finally, the continuum interface model will be implemented in a code that is used by the industry for the study of the influence of metallic interfaces at a homogenized material point (engineering) level, or microdevice (e.g. thin film or micro-scale interconnect).
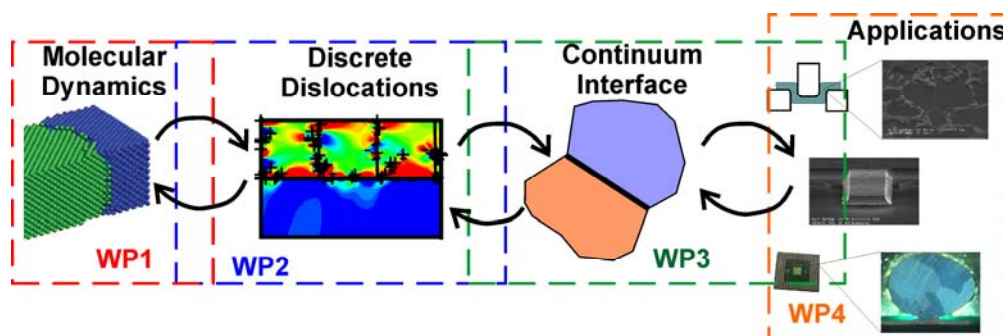

Figure 1. *Scales, methodologies and scale transitions up to the applications level, addressed in this project*

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Within the generic framework defined above, a carrier problem will be addressed, which is the plasticity at large angle grain boundaries up to the level of void nucleation through the accumulation of dislocations at the interface. The choice for this particular carrier is dictated by its exceptional complexity on the one hand, and the availability of experimental observations on the other hand, e.g. [61,68,71].

3.2 Multi-scale character

This project addresses several length scales and involves different research groups having individual expertise at each of these levels. The project aims to establish a truly multi-scale approach, by focusing on the following 3 scale transitions, as illustrated in the figure above:

- Transitionmolecular dynamics – discrete dislocations: this will be carried out by developing coarse-grained constitutive rules for the DD simulations. Quantification and validation of these rules is done on the basis of the computed MD response.

- Transition discrete dislocations – continuum interface: this will be carried out using 2 concurrent approaches. First, an interfacial computational homogenization framework will be set up that links a DD volume to a continuum interface response. Parallel to this, explicit constitutive equations will be developed for a continuum interface element, for which the earlier computed interface response serves as a reference.

- Transition interface – full finite element simulation: this will be carried out by implementing the interface element in an RVE of polycrystals or a full finite elementmodel of a microdevice. To upscale the response of the RVE, a standard computational homogenization framework will be used.

3.3 Expertise of the research team

The project unifies disciplines in mechanics, physics and materials science, which is a prerequisite to address all the scales of interest. Each of the participating groups has its scientific strengths in one of these disciplines, which will be integrated through the scale transitions to be made:

- Research group of prof.dr.ir. E. van der Giessen has a strong international expertise in discrete dislocation modelling, both in 2D and 3D: (1) development of DD methodology for boundary-value problems [8,15,54]; (2) application to microstructure evolution problems [2,4,45], technological problems involving (sub-)micron scale plasticity in confined volumes [5,17-20,46,47,49-51,55], and (interfacial) failure [3,14,16,32]; (3) substantiation of higher-order crystal plasticity theories [9,31,52].

- Research group of prof.dr.ir. M. Geers: A solid expertise has been built up in this group in a number of topics that are relevant for this project, i.e. (1) enhanced crystal plasticity models that constitute the adjacent continuum nearby an interface [6,7,23-25,28,29]; (2) characterization of interface models [11-13,22]; (3) computational homogenization (coarse graining) of continua across scales [26,27,37-40]; (4) reliability in lead-free solders, emphasizing the role of interfaces [1,21,41,42].

- Research group of prof.dr. B. Thijsse: This group is part of the Virtual Materials Laboratory in Delft and has considerable experience in Molecular Dynamics modeling of metallic interfaces [10,35], dislocations [33,34] and grain boundaries [36] in ultrathin films, and in constructing interatomic Embedded-Atom type potentials by fitting the relevant parameters to crystal structure, elastic constants, etc, and to results from first-principles calculations. Computational visualisation and analysis tools, as well as a highly promising mixed Molecular Dynamics + Monte Carlo code are available. Dr. L. Nicola has expertise in two topics relevant to the proposed research: DD plasticity (applied to thin films and interconnects [49,50]), and (strain gradient) crystal plasticity [52,53].

3.4 Short description of workpackages and PhD vacancies

As a carrier, the complex problem of unstructured large angle grain boundaries will be used. The work in this project is organised in four interrelated workpackages (WPs).

WP1: Molecular dynamics analysis (vacant PhD position at TU Delft, contact professor Barend Thijsse)
This work package is fully directed towards supplying the relevant data at the smallest scale, needed to fill in and drive the DD modelling. It is here that the interaction between dislocations and grain boundaries (impact, dissolution, re-nucleation, void nucleation upon multiple dislocation arrival) will be studied at the greatest detail, for various types and orientations of grain boundaries, and for various key material properties involved (elastic constants, etc). We will perform systematic studies of the influence of these parameters on the dislocation/grain boundary behaviour and extract "phase diagrams" for the different effects that will occur. Critical values of the local stress tensor and/or energy will be a second important part of the output of this work package, as input for WP2. The sensitivity with respect to the lattice properties will be explored in the final stage of this WP.

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Required background for the PhD position in WP1:
MSc. in materials science, physics, chemistry, or mechanical engineering, with a good background in solid state science/engineering. Programming experience required. Experience in molecular dynamics and affinity with computer modeling are strong plus points.

WP2: MD-DD scale transition & Discrete dislocation dynamics analysis (vacant PhD position at RU Groningen, contact professor Erik van der Giessen)

This workpackage will be devoted to the development of numerical tools to incorporate the storage of dislocations in GBs and their nucleation from boundaries and interfaces. Like other treatments of short-range interactions, these tools will have the form of constitutive rules in terms of Peach-Koehler forces, resistances and probabilities. The work will supplement ongoing activities to implement the transmission of dislocation glide across small-angle GBs. The rules for storage will, ultimately, also lead to criteria for the onset of voiding at the interface. As a proper criterion for homogeneous dislocation nucleation is still pending, it is likely that a few criteria (e.g., energy, stress or stress-gradient based) will have to be postulated and subjected to validation of the DD concepts by appropriate MD simulations (WP1). The latter will also provide the values of the DD parameters for a specific class of boundaries/interfaces (i.e. MD-DD scale transition). The other scale transition, to the continuum scale, will be based on a large number of DD simulations, required to help develop the continuum model in WP3 and to provide that model with appropriate material parameters.

Required background for the PhD position in WP1:
MSc. in materials science or (applied) physics with a background in solid mechanics, or MSc. In mechanical (or aeronautical) engineering with a good background in metallurgy, and solidmechanics. Hands-on experience in discrete dislocation dynamics is not necessary but a strong plus point.

WP3: DD-CM scale transition & Continuum interface analysis (vacant PhD position at TU Eindhoven, contact professor Marc Geers)

This workpackage will focus on two main tasks aiming to establish a scale transition link between the DD simulations and continuum interface modelling. First, a generic computational homogenization framework will be developed that links a DD volume to an entirely numerical continuum interface response. Dedicated scale transition relations will have to be established that will properly define the boundary value problem for the DD analysis and extract the overall interface response in a consistent manner. Parallel to the numerical upscaling, a coarse grained interfacial element description will be developed, with particular (parameterized) constitutive properties. In the first stages, it will neighbour continuum elements that transport plasticity through dislocations towards the interface, which will lead to a stress interaction and dislocation evolution at the interface. The interface should therefore provide the constitutive behaviour that affects the adaptive boundary conditions of the adjacent continuum. A higher-order interfacial description, which is compatible with state-of-the-art continuum description of the neighbouring elements will therefore be a prerequisite (see relevant work of the applicants [24,25,56-59]). The generic scale transition framework will be applied to the carrier problem, for which the corresponding DD model will be provided by WP2. The results of this computational homogenization analysis will serve as a reference for development of explicit constitutive equations for a continuum interface element.

Required background for the PhD position in WP3:
MSc. in mechanical engineering with a strong background in computational mechanics and mechanics of materials (or MSc in materials science with a strong background in modeling). Experience in micromechanics of metals, modeling at the microstructure level, and associated microstructural finite element techniques are important plus points.

3.5.4 WP4: Scale transition CM-applications (contributions from Corus, NXP and Philips)

This workpackage will concentrate on the last scale transition and the utilization of the interface computational description developed to the benefit of the industrial simulation practice.

5. Literature

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