Multiscale integrated interface Modelling – Mi2M

STW-project in the programme Multi-Scale Simulation Techniques
A multi-scale approach towards integrated cohesive interface elements

Participating groups
Prof.dr.ir. M.G.D. Geers (contact m.g.d.geers@tue.nl)
Department of Mechanical Engineering (ME), Eindhoven University of Technology (TU/e–ME)
Section Mechanics of Materials

Dr.ir. P.J.G. Schreurs, Dr.ir. L.E. Govaert (contact p.j.g.schreurs@tue.nl)
Section Polymer Technology (TU/e–PT)
Department of Mechanical Engineering (ME), Eindhoven University of Technology (TU/e)

Prof.dr.ir. E. van der Giessen (contact E.van.der.Giessen@rug.nl)
Department of Applied Physics, University of Groningen (RuG–Phys)
Micromechanics of Materials

Vacancies (1 PhD / 1 Post-Doc)
1 PhD vacancy at the Eindhoven University of Technology
1 Post-Doc vacancy at the University of Groningen

1 Summary
Cohesively bonded interfaces play a dominant role in a variety of products, commonly based on thin film coated substrates or layered thin film structures. The reliability of such products and devices is often compromised by the occurrence of interfacial separation processes (or delamination). Dedicated experiments to measure interface performance are being developed in industry and academia, but the results clearly reveal that a macroscopic approach to this problem does not enable the development of truly predictive insights under different loading conditions. The key problem resides in the fact that the total fracture energy encompasses contributions from physical debonding processes and micro-scale dissipation processes in the bonded material, which cannot be separated without a multi-scale approach. Due to this lack of insight, the industry is largely relying on trial-and-error procedures for each interfacial system to be designed or optimized.

This project focuses on a generic multi-scale approach that bridges molecular processes (de-adhesion, chain pull-out and scission and micro-dissipation) to a coarse scale description by means of enriched cohesive zones. A fine scale representation of the interface will be established, including geometrical and physical defects, which will feature the competition between de-adhesion and micro-deformation. Dedicated molecular mechanisms will be coarse grained to the fine scale model, where temperature-, pressure-, rate- and time-dependent continuum behaviour will be incorporated. The scale transition to the cohesive zone level will be established in a two-step manner, (i) by means of a rigorous, entirely computational homogenization scheme, from which (ii) a closed-form description of the cohesive zone will be extracted. With the obtained generic structure of the cohesive zone model, more complex loading conditions can be handled.

2 Research team
The research team applying for this research project consists of 2 academic and 4 industrial partners from different sectors. The academic partners are sharing their expertise, relying on their individual strengths on modeling at two distinct length scales, whereas the mutual co-operation will provide the input needed to establish the scale transitions. The industrial partners unify a common interest in the behaviour of cohesive interfaces, each from their own application perspective. The proposed team therefore gathers the required scientific expertise and the generic industrial interest, which is needed to achieve the goals of this project as a part of the MuST programme. The role of each of the partners and staff members involved is listed below.
3 Scientific project description

3.1 Introduction and objective
Cohesively bonded interfaces play a dominant role in a variety of products, commonly based on thin film coated substrates or layered thin film structures. The thickness of the films or layers often is in the range of 30 nm up to 100 μm and more. The cohesively bonded systems of interest for this project typically involve two different polymers, or a polymer and a substrate of a non-polymeric material e.g. a metal, glass or silicon. The adhesion between the layers in such systems has been the subject of great scientific and industrial interest over the past decades [Lane, 2003; Singhe and Gratien, 2003]. Most work has been focussed onto brittle interface failure in metal/metal and metal/ceramic interfaces. Ductile failure has been studied by taking into account the (visco)plastic dissipation mechanisms in the adjacent materials [Mishnaevsky and Gross, 2005]. Ductile adhesive failure has been investigated using classical fracture mechanics with small scale yielding [Hui et al., 1992; Lane et al., 2000; Saulnier et al., 2004]. The interaction between adhesive and cohesive failure has only recently given some attention [Yao and Qu, 2002]. A systematic approach addressing the relevant scales separately and mutually seems to be missing however.

The classical reasoning in addressing the problem is to study the adhesion on the basis of the physicochemical bonding of the layers at the separating interface. Whereas this provides clear answers in brittle interfaces, it constitutes a major problem for cohesive interfaces. The main reason for this, is that during interfacial separation (or delamination), a considerable amount of energy is dissipated in deforming the adjacent material. As a result, different experimental set-ups do not provide consistent measurements of the work of adhesion, since the measured fracture energy consists of a contribution from (1) actual debonding at the surface, (2) dissipative deformation in the bonded material adjacent to the interface and (3) the interaction between both previous mechanisms. A typical example of this is the measured work of separation in e.g. a polymer-coated metal, where values of 2 J/m² [Fedorov et al., 2007], 30 J/m² [van Tijum et al., 2007] and 194 J/m² [van den Bosch et al., 2007] have been reported by different techniques on exactly the same material system. The physicochemical bonding was expected to be largely identical in each of the tests used, but the micro-scale dissipation enforced in each was substantially different. At this point, the scientific community cannot provide predictive values for each situation and the industry is largely relying on trial-and-error procedures for each interfacial system to be designed or optimized.

In the particular example studied by Van den Bosch et al. [2006,2007] it has been demonstrated that the fine scale dissipation mechanism nearby the interface was fibrillation. Delamination comprised various failure processes, including extending fibrils, de-adhesion from the surface and even breakdown of fibrils. The latter mechanism typically involves the pull-out and scission of molecular chains. At the continuum interface level, all these mechanisms result in an overall work of separation that is larger than the classical adhesion energy by an amount equal to the mechanically induced dissipation near the interface. Using a coarse scale description of an interface, the fine scale dissipation cannot be discriminated from the role of the adhesion, thus rendering the resulting models intrinsically case-specific.

In order to overcome this problem, a multi-scale simulation method is inevitably required.

Objective
This project focuses on the development of a multiscale tool that enables the identification and integration of the interaction between adhesion and micro-scale dissipation in an upscaled cohesive interface description.

3.2 Multi-scale character
As emphasized above, the interplay between the loss of adhesion and micro-scale dissipative mechanisms cannot be tackled without making use of an integrated multi-scale approach. This project essentially addresses three interacting length scales:

- The molecular level, needed to assess the dissipative contribution of bonding structures that are too small to fit in a continuum approach.
- The fine scale interface level, at which a detailed continuum model will be used to capture the influence of a distributed adhesion, and irregularities and defects at the level of the bonded interface.
- The macroscopic level, in which the mechanisms identified at the fine scale will be modelled at a constitutive level in terms of bulk constitutive properties and cohesive zone models.
Two scale transitions are required. The first one relies on the coarse graining of the molecular results, which will be used in the failure model at the fine scale model. The fine scale model, with a considerable level of physical and geometrical complexity, will be homogenized to the coarse scale, using a direct computational method [Kouznetsova et al., 2001, 2002, 2004], specific for the type of interface studied here.

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 are to be integrated through the scale transitions to be made:

- 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) numerical-experimental characterization of interface models for polymer-coated metal sheet [van den Bosch et al., 2006, 2007]; (2) modelling of damage in continua, both using quasi-brittle and ductile enriched models (3) computational homogenization (coarse graining) of continua across scales [Kouznetsova et al., 2001, 2002, 2004; Geers et al., 2001, 2003].

- Research group of Dr.ir. P.J.G. Schreurs and Dr.ir. L.E. Govaert: This group has a long-standing expertise in the industrial arts of manufacturing polymer-based products, with a special emphasis on bridging the gap between science and technology in the area of polymer processing and design. The three-dimensional non-linear viscoelastic constitutive equations are derived and improved on the basis of experimental observations and include yield, intrinsic strain softening, strain hardening and the important dependence on strain rate and temperature [van Melick et al., 2002; Meijer et al., 2003, 2005; Klompen et al., 2005]. These models are here required at the level of the fine scale interfacial model.

- Research group of prof.dr.ir. E. Van der Giessen: This group has been working on various aspects of polymer modelling inspired directly by physical mechanisms. Landmark results relevant for this project include the full-network model for rubbers [Wu and Van der Giessen, 1993], the first physically-based cohesive zone model for crazing in polymers [Tijssens et al., 2000, 2002; Basu et al., 2005], micromechanical studies of void growth in polymers and blends [Steenbrink et al., 1997, 1998, 1999; Pijnenburg et al., 1999, 2005] and extensive study of the fracture of homopolymers [Estevez et al., 2005]. In more recent years, the group has been involved in coarse-grained molecular dynamics simulations of glassy polymers, including in particular the analyses of de-bonding of two glassy polymers glued together by stitching (bi and tri-block) co-polymers [Bulacu, 2008; Bulacu and Van der Giessen, 2005, 2007].

3.4 Short description of workpackages and vacancies

The work in this project is organised in four workpackages (WPs).

WP1: Coarse-grained molecular dynamics analysis (vacant Post-Doc position at RU Groningen, contact professor Erik van der Giessen)

Recent work by Ph.D. student Bulacu in Groningen has concentrated on computing the work of adhesion provided by block co-polymers that stitch together two immiscible polymers [Bulacu, 2008]. The coarse-grained molecular dynamics model was designed so that only the work is computed that is done while the stitching molecules are being pulled out. This has yielded an improved understanding of forced reptation and some interesting scaling relations. In the present workpackage, this will be extended by allowing for concurrent relaxation processes in the tails to take place. This will couple chain pull-out to large scale viscoelasticity, including the possibility of shear yielding and crazing, while comparison with the previous results provides information in how the total fracture energy can be attributed to the various mechanisms. The coarse-grained results will be used in the fine scale continuum model, in particular where the molecular mechanisms described above are not well addressed through the bulk equations used. Two types of systems are relevant here: (1) a polymer–polymer system, and (2) a polymer perfectly adhering to a rigid
substrate (e.g. metal), where pull-out and chain scission occurs due to its strong bonding to the substrate (the latter is typically observed in polymer-coated steel, as used by Corus).

**Required background for the Post-Doc position in WP1:**
PhD in mechanical (or aeronautical) engineering, materials science or (applied) physics related to the micromechanics of polymers. Experience with molecular dynamics simulations is not required but would be a strong plus point.

**WP2 & WP3: Fine scale interface modelling, interfacial homogenization & coarse scale cohesive description (vacant PhD position at TU Eindhoven, contact professor Marc Geers)**
While WP1 focuses on the molecular dissipation processes, the fine scale model will address the dissipation and delamination processes on the length scales of fibrils (figure 1), including void formation, fibril extension, etc. The failure behaviour of individual fibrils, either through brittle fracture or stable necking, will be determined making use of the advanced constitutive models developed (and experimentally verified) in previous [Klompen et al., 2005; Meijer et al., 2003,2005] and ongoing work.

![Figure 1](image)

**Figure 1. Typical example of an interfacial separation problem that emphasizes the interaction between the loss of adhesion and dissipation near the interfaces [van den Bosch et al.].**

**Model features:**

- The interface will be modelled with a varying degree of geometrical imperfections (roughness, spatially distributed bonding).
- Different loading configurations will be applied to the interface (tension/compression/shear, with different pressures, temperatures, strain rates and ageing history).
- State-of-the-art 3D nonlinear visco-elasto-plastic continuum models will be applied at the fine scale model, enriched with a damage model to describe the failure and dissipative processes.
- The nucleation and growth of voids at the interface will be incorporated.
- The constitutive description of failure processes in the bonded polymer or fibrils, which is not accounted for in existing bulk models, will be determined by coarse graining the molecular results of WP1.

A fine scale model of the type suggested in WP1 provides a detailed insight in the intrinsic role of several interfacial characteristics. Yet, it cannot be used for practical engineering applications, where the interfaces of interest are subjected to real macroscopic loads (e.g. rolling/bending/shearing for systems-in-foil, displays and solar cells; bending/deep-drawing/wall-ironing for polymer coated metal sheet; extension for stretchable electronics). WP3 therefore addresses the scale bridging to this macroscopic scale. At this level, we depart from the recent experience in the PhD work of Van den Bosch, where cohesive zones were developed and characterized with peel tests for PET-coated steel. This workpackage will apply and enrich the computational homogenization model developed in the Mechanics of Materials group, to extract a realistic macroscopic behaviour. The result thereof will be used to develop an updated 3D cohesive zone model, which carries the main fine scale characteristics that impact the coarse scale.

**Required background for the PhD position in WP2/3:**
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.

**WP4: Industrial support – experimental data / validation / implementation**
This workpackage integrates the industrial support in the project and defines the transfer of results.
7. Literature

7.1 Relevant publications from the research group (last 6 years)
M.G.A. Tijssens and E. van der Giessen, Polymer 43, 831-838 (2002).

7.2 Other references related to this research project