Modeling, Control and Opportunities of Mechanical Interfaces Across the Scales

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Dr.-Ing. Patrick Kurzeja

aus Bochum

Kommissionsvorsitz:	Prof. Dr.-Ing. habil. J. Mosler
Referiert durch:	Prof. Dr. Anna Pandolfi
	Prof. Stanisław Stupkiewicz, PhD, DSc
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Preface

The research presented in this contribution was mainly conducted at the Institute of Mechanics at TU Dortmund University, where it finally obtained its current focus, shape and depth. Some parts were also conducted during stays (in chronological order) at the Chair of Continuum Mechanics at Ruhr-University Bochum, the School of Engineering and Applied Sciences at Harvard University, the Statistical Physics group at the University of Duisburg-Essen and the group of Technical Mechanics - Structural Mechanics at the University of Bremen. It would not have been possible without the valuable contributions from colleagues affiliated (at that time). The support of colleagues, friends and family is highly, cordially and warmly acknowledged.

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"Not all questions are answered,
but fortunately some answers are questioned."

Terry Pratchett

Abstract

This treatise analyzes various roles of mechanical interfaces in natural and artificial environments. From the classic perspective of spatial scales, the chapters evolve from modeling at the atomistic scale, to single continuum interfaces to larger systems of interfaces. They will cover molecular descriptions, sharp and diffuse interface models as well as effective ensemble properties. From the perspective of control, they evolve from naturally arising to artificially created objects. Freely evolving cracks, phase changes and interface design for controlled fluid-structure interaction will be shown for illustration. From the perspective on new opportunities, finally, they evolve from risk-bearing imperfections to technical and scientific opportunities. While damage is investigated as a typical risk scenario, novel potentials will be explored for non-destructive characterization, low-frequency attenuation and information enhancement for artificial neural networks.

Publication notice

The extended summary of research findings presented in this contribution is based on the following publications (in chronological order):

- P. Kurzeja. The criterion of subscale sufficiency and its application to the relationship between capillary pressure, saturation and interfacial areas. *Philosophical Transactions of the Royal Society A*, 472: 20150869, 2016. doi:10.1098/rspa.2015.0869.
- T. Cohen, P. Kurzeja and K. Bertoldi. Architected squirt-flow materials for energy dissipation. *Journal of the Mechanics and Physics of Solids*, 109: 22-33, 2016. doi:10.1016/j.jmps.2017.08.003.
- K. Schröer, P. Kurzeja, S. Schulz, P. Brockmann, J. Hussong, P. Janas, I. Wlokas, A. Kempf and D. Wolf. Dilute suspensions in annular shear flow under gravity: simulation and experiment. *EPJ Web of Conferences*, 140: 09034, 2017. doi:10.1051/epjconf/201714009034.
- C. Sievers, J. Mosler, L. Brendel and P. Kurzeja. Computational homogenization of material surfaces: From atomistic simulations to continuum models. *Computational Materials Science*, 175: 109431, 2020. doi:10.1016/j.commatsci.2019.109431.
- C. Sievers, J. Mosler and P. Kurzeja. Projection vs. relaxation of adjacent bulk deformation for surface modeling: Theoretical and numerical aspects. *International Journal of Solids and Structures*, 226: 111084, 2021. doi:10.1016/j.ijsolstr.2021.111068.
- A. Bartels, P. Kurzeja and J. Mosler. Cahn-Hilliard phase field theory coupled to mechanics: Fundamentals, numerical implementation and application to topology optimization. *Computer Methods in Applied Mechanics and Engineering*, 383: 113918, 2021. doi:10.1016/j.cma.2021.113918.
- T. Heitbreder, P. Kurzeja and J. Mosler. On general imperfect interfaces with spatially non-constant displacement jumps. *International Journal of Solids and Structures*, 232: 111068, 2021. doi:10.1016/j.ijsolstr.2021.111068.
- K. Langenfeld, P. Kurzeja and J. Mosler. How regularization concepts interfere with (quasi-) brittle damage: a comparison based on a unified variational framework. *Continuum Mechanics and Thermodynamics*, 34: 1517-1544, 2022. doi:10.1007/s00161-022-01143-2.
- P. Kurzeja and H. Steeb. Acoustic waves in saturated porous media with gas bubbles. *Philosophical Transactions of the Royal Society A*, 380: 20210370, 2022. doi:10.1098/rsta.2021.0370.
- K. Langenfeld, P. Kurzeja and J. Mosler. On the curvature dependence of gradient damage models: Control and opportunities. *Computer Methods in Applied Mechanics and Engineering*, 410: 115987, 2023. doi:10.1016/j.cma.2023.115987.

- P. Kurzeja and B. Quintal. Harnessing local flow in buckling pores for low-frequency attenuation. *International Journal of Solids and Structures*, 285: 112508, 2023. doi:10.1016/j.ijsolstr.2023.112508.
- G.-L. Geuken, J. Mosler and P. Kurzeja. Incorporating sufficient physical information into artificial neural networks: a guaranteed improvement via physics-based Rao-Blackwellization. *Computer Methods in Applied Mechanics and Engineering*, 423: 116848, 2024. doi:10.1016/j.cma.2024.116848.

Contents

1 Introduction

1.1 The aim of this work

The aim of this work is to provide a view on mechanical interfaces that does not only describe their mechanical behavior — but to highlight the opportunities that arise from them as well. Voids, cracks and imperfections, for instance, may pose a challenge in terms of uncertainty and safety, on the one hand. On the other hand, though, a smart arrangement of cavities may turn instabilities into attenuating materials, surface energies may guide topology optimization and interfacial areas may provide sufficient information on the underlying structure.

Of course, it is an impossible task to give equal consideration to all possible research areas of interfaces within or between the individual disciplines. The mechanics of interfaces is found, for instance, in fracture mechanics [34, 102], crystal plasticity [169], fluid-structure interaction [209], capillarity and wetting [57], porous media [20] and granular media [123], to name only a few. Even more so, the mechanics of interfaces connects to interfacial chemistry [247], molecular physics [81, 121], biology [154] and medicine [162, 241, 246]. Also materials with internal interfaces are numerous, including metals [150], glass [35], polymer powders [9], foams [92], soil [235], paintings [146], food [245] and many more. The present examination hence cannot cover all such fields, let alone the various developments in theory, simulation and experiment. Some of them will be touched only briefly or implicitly. References are also chosen to cope with the respective focus of each section, trying to avoid redundancy. This should by no means be understood as a judgement of relevance. Self-contained articles will moreover provide a detailed view on selected higlights by concluding individual sections.

The present treatise will hence combine material modeling and numerical analyses of mechanical interfaces along six chapters with a focus on continuum mechanics modeling. Chapters 1 and 2 will establish an overview of the interface's roles and formulations and a link from atomistic to continuum descriptions. Chapters 3 and 4 discuss the numerical modeling of sharp and diffuse interfaces, respectively. Chapters 5 and 6 will eventually demonstrate how interfaces can be used for the design of structures and as a source of information. Each chapter starts with a general introduction and concludes with selected in-depth articles.

The order of the present treatise can be read and interpreted in three different ways:

- modeling interfaces across the length scales,
- control of interfaces,
- opportunities of interfaces.

From the classic perspective of spatial scales, the chapters evolve from modeling at the atomistic scale, to single continuum interfaces to ensembles of interfaces. They will cover molecular descriptions, sharp and diffuse interface models as well as effective ensemble properties. From the perspective of control, they evolve from naturally arising to artificially created objects. Freely evolving cracks, phase changes and interface design for controlled fluid-structure interaction will be shown for illustration. From the perspective on their potential impact, finally, they evolve from risk-bearing imperfections to technical and scientific opportunities. While damage is investigated as a typical risk scenario, novel potentials will explored for destructive-free characterization, low-frequency attenuation and information enhancement for artificial neural networks.

1.2 Roles of mechanical interfaces and surfaces

Before turning the view towards a specific scientific description, possible roles of mechanical interfaces shall first be reviewed with respect to characteristic mechanisms in natural and artificial environments. They range from plants, soil and tissues to machining tools and haptic devices [40, 130, 140, 154, 164, 235, 242]. These roles, whether intended or not, help to understand the motivation for the plurality of scientific developments. A preferential classification of such roles, again, is difficult to determine due to the various disciplines involved. For illustration, the following introduction will classify some of the most prominent variables in continuum mechanics: motion, mass, stress, and energy. A more comprehensive discussion of interface variables can be found in the next chapters.

The probably simplest and most intuitive role of an interface is that of a mere two-dimensional boundary between two three-dimensional domains. Assuming pure geometrical objects yet without mechanical properties, they naturally appear as soon as two materials have to be distinguished. This includes, for instance, a distinction between crystals of different orientations [169], phase boundaries [57, 112] or composite materials [44]. Contact problems pose another technically relevant challenge, e.g., for wheel-rail contact in railway engineering [153], wear of engineering materials [128] or microcrack-closure-reopening mechanisms in damage mechanics [74]. The analysis of interfaces as geometrical objects has a strong connection to the mathematical fields of differential geometry [229] and topology with applications to computational visualization and mesh generation [257]. They can also be understood as a part of more generalized geometric objects, e.g., submanifolds that also cover contact lines or contact

points or interfaces of higher-dimensional spaces. The present focus will nevertheless remain on two-dimensional, mostly continuously differentiable manifolds embedded in three-dimensional space or, for some simplified studies, one-dimensional manifolds in two dimensions.

To clarify terminology, a surface is considered to be a special case in the present context of interfaces, i.e., an interface that confines a single material but is adjacent to no other or to vacuum, respectively [147]. Very often, surrounding materials with negligible mechanical impact motivate the terminology of surfaces as well, e.g., ambient air that negligibly contributes to deformation processes in a solid part. Even more so, slender structures such as layers, shells, plates or membranes may be considered to fall under the terminology of interfaces. This terminological link is less common if these elements appear alone, e.g., as a single membrane. The description of slender structures as interfaces may nevertheless be possible if they interact mechanically with a surrounding material, e.g., in composite materials [13] or aircraft [191]. For the sake of brevity, the term interface shall hence also be understood as a generic term to imply surfaces, layers, plates, membranes, films, coatings, etc. Specific terms will be used when the context clearly suggests its use, e.g., in terms of specific applications, material models or numerical implementations.

Having defined a purely geometrical role, the motion of interfaces can furthermore add dynamic aspects to their investigation. Interface nucleation and growth, as two particular cases, are responsible for the initial stages of phase transformations or damage evolution [45]. Deformable interfaces can also be used to guide signals in the bulk materials or for the characterization of the microstucture that relates to the dynamic response [163]. Moving interfaces, even without any change of their initial shape, can support transport processes such as those of colloids [23] or gas bubbles [57]. Finally, the static case can be the result of optimization strategies with transient interface evolution in natural and artificial structures.

A first non-kinematic property that can be assigned to interfaces is mass. Interfaces with mass are prominent in design principles of light-weight structures such as constructions with shells and plates [8, 191]. Also organic materials such as lipid layers [120] are governed by the available mass for the creation of interfaces [178]. Consequently, theoretical and numerical descriptions account for that mass to calculate weight due to gravity or inertia in resonance analyses. In addition to possessing mass, interfaces can also act as a mass storage, e.g., for pollutants [82], surfactants [143], adsorption of tin molecules [99], diffusion [202], absorption processes [227] or in catalyst design [86].

The assumption of an ideal two-dimensional geometrical entity must be questioned at the latest, however, when considering their property of mass. Practical interfaces of course have a finite width, e.g., the transition zone between two states of matter [182] or the human skin [24]. In many cases, though, the zero-thickness assumption is a valid and useful approximation. Interfaces will hence be indealized as two-dimensional objects in most of the following chapters. The validity of this assumption will yet be called into

question at two later stages, the upscaling of molecular surfaces and the zero-thickness limit of numerical descriptions of diffuse interfaces.

Stress is another, if not the most prominent, mechanical property that can be assigned to interfaces and directly interferes with the possession and exchange of momentum. Slender components can allow for very ressource-efficient design, alone and as part of a sandwich construction [77]. The stresses in slender components are typically caused by two types of deformations, in-plane strain and curvature-related bending [8], which became manifest in the well-established theories of plates and shells. Another special case of interface stress is the so-called surface tension, which is responsible for capillary effects [57]. Unlike classic elastic solids, its (true) interface stress value remains constant in the deformed configuration. Stresses normal to the interface, in contrast, are vital for interfaces connecting different materials such as soldered connections and glued joints [91], gecko spatulae [100] or protecting interfaces such as capsules [95]. Interface stresses also significantly affect the dynamic behavior, e.g., in contact zones for ultrasound transmission [199], slip and mobility at boundaries [137, 215] or the exchange of momentum and angular momentum of microswimmers [22, 72].

Interfaces can also possess and exchange energy, having their own temperature and entropy, accordingly. Control of radiation and insulation are hence interface-dominated applications [145]. The interplay between interface energy and bulk energy moreover yields scale effects to weaken or to strengthen the homogenized system [132]. Energy dissipation can also be used for the characterization of the interfaces' size or shape. Destruction-free ultrasound testing, for instance, can help to relate frequency-dependent attenuation to the interface structure [163]. Fracture toughness and tearing is also directly related to the energy required to form free surfaces [101, 213]. Their role as energetic boundaries for mechanical and chemical processes makes interfaces relevant for the performance of structural batteries as well [240].

Eventually, there is no interface without a surrounding bulk space. The roles of interfaces are hence quite often not defined by themselves alone, but rather by their effect on the surrounding system. Crack propagation poses a serious thread to the reliability of machines, the interfacial area of lungs determines their functionality and the shape and arrangement of cavities can tip the balance between stable and instable structures. The presence of mechanical interfaces implies a change of the adjacent bulk phase for better or worse. The following investigation thus aims at exploring their modeling, their control and their opportunities.

1.3 Introduction to continuum formulations of interfaces

The following formulation establishes an initial terminology via a basic interface model. It shall help to better follow the next chapters and to connect them to established models. Nomenclature and terminology may slightly differ between the in-depth articles within this treatise. They follow the scientific conventions of the respective (sub)areas

of research. The difference is yet considered small, while symbols and wording remain as close as possible to standard conventions.

1.3.1 Interface geometry and kinematics

Unlike bulk materials, interfaces can undergo deformations into the embedding higher-dimensional space. This opens possibilities that are special to systems with interfaces such as creasing, folding, debonding or curvature effects. Some of the most relevant properties of interface kinematics shall be introduced by assuming a well-defined parameterization of the interface by curvilinear coordinates $\{\theta^1, \theta^2\}$. With the placement of a material point $\boldsymbol{X}$ in the initial configuration and $\boldsymbol{x}$ in the deformed configuration, the tangent space of the interface can be spanned by covariant tangent vectors $\boldsymbol{G}_\alpha = \partial_{\theta^\alpha}\boldsymbol{X}$ and $\boldsymbol{g}_\alpha = \partial_{\theta^\alpha}\boldsymbol{x}$, respectively, with $\alpha \in \{1, 2\}$. For the sake of brevity, not all following relationships are formulated for the initial configuration (indicated by capital symbols) and the deformed configuration (indicated by lower case symbols). The inner product of the covariant tangent vectors yield the metric coefficients $\boldsymbol{g}_\alpha \cdot \boldsymbol{g}_\beta = g_{\alpha\beta}$ or the so-called first fundamental form of the interface. The normal vector can accordingly be defined by $\mathbf{n} = \boldsymbol{g}_1 \times \boldsymbol{g}_2 / |\boldsymbol{g}_1 \times \boldsymbol{g}_2|$. A dual basis is moreover defined by the contravariant basis vectors $\boldsymbol{g}^\alpha$ via the Kronecker delta as $\delta^\alpha_\beta = \boldsymbol{g}^\alpha \cdot \boldsymbol{g}_\beta$.

The standard identity mapping for the interface

$$\overline{\boldsymbol{I}} = \boldsymbol{I} - \boldsymbol{N} \otimes \boldsymbol{N} = \boldsymbol{G}_\alpha \otimes \boldsymbol{G}^\alpha, \quad \overline{\boldsymbol{i}} = \boldsymbol{i} - \boldsymbol{n} \otimes \boldsymbol{n} = \boldsymbol{g}_\alpha \otimes \boldsymbol{g}^\alpha$$

is a key property for the projection onto the interface plane. In the case of interfaces following the bulk deformation, it isolates the interface deformation from the bulk deformation state. This is the case for many mechanical interfaces such as cracks and phase boundaries. Exceptions can nevertheless be found, for instance, during phase changes or for coatings that detach from the underlying solid. For interfaces attached to the bulk motion, the deformation gradient $\boldsymbol{F}$ with $\mathrm{d}\boldsymbol{x} = \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{X}$ can be transformed into an interface deformation gradient by $\overline{\boldsymbol{F}} = \boldsymbol{g}_\alpha \otimes \boldsymbol{G}^\alpha = \boldsymbol{F} \cdot \overline{\boldsymbol{I}}$. The right Cauchy-Green tensor $\boldsymbol{C} = \boldsymbol{F}^T \cdot \boldsymbol{F}$, as another example, transforms accordingly via $\overline{\boldsymbol{C}} = \overline{\boldsymbol{F}}^T \cdot \overline{\boldsymbol{F}} = \overline{\boldsymbol{I}} \cdot \boldsymbol{C} \cdot \overline{\boldsymbol{I}} = g_{\alpha\beta}\, \boldsymbol{G}^\alpha \otimes \boldsymbol{G}^\beta$. In-plane strains of an isotropic interface can then be characterized by the principal invariants of the interface right Cauchy-Green tensor, $I_{\overline{C}} = \overline{\mathrm{tr}}(\overline{\boldsymbol{C}}) = \overline{\boldsymbol{C}} : \overline{\boldsymbol{I}}$ and $II_{\overline{C}} = [I^2_{\overline{C}} - \overline{\mathrm{tr}}(\overline{\boldsymbol{C}}^2)]/2$.

Curvature is another key property that is characteristic for interfaces and their role as submanifolds. It relates to bending of slender structures, for instance. The covariant coefficients of the curvature tensor define the second fundamental form of the interface, $\boldsymbol{k} = -\overline{\nabla}\,\mathbf{n}$. The mean curvature can be defined as $\kappa = -\frac{1}{2}\overline{\nabla} \cdot \boldsymbol{n}$, while definitions with respect to sign and prefactor may differ in some literature. The surface divergence theorem is an interesting result, which underlines the peculiarity of interfaces. It relates the divergence of a vector-valued field not only to the flux across the interface boundaries (in tangent normal direction at the boundary edge $\overline{\boldsymbol{n}}$) but also to its curvature as a flux

outside the curved interface into the embedding space (last term in the subsequent equation, which does not appear for mere bulk volumes)

$$\int_{\mathcal{A}} \overline{\nabla} \cdot \bullet \, \mathrm{d}a = \int_{\partial\mathcal{A}} [\bullet \cdot \overline{\boldsymbol{n}}] \, \mathrm{d}c - \int_{\mathcal{A}} \kappa [\bullet \cdot \boldsymbol{n}] \, \mathrm{d}a.$$

1.3.2 Prominent effects by the example of elastic interface energy

Considering purely elastic deformations, the total elastic energy of the system shall be split into an integral over the initial bulk domain $\mathcal{B}_0$ and the initial interface domain $\mathcal{A}_0$

$$\Psi_{\mathrm{tot}} = \int_{\mathcal{B}_0} \psi_V \, \mathrm{d}V + \int_{\mathcal{A}_0} \psi_A \, \mathrm{d}A.$$

Bulk energy ψ_V can depend on deformation gradient $\boldsymbol{F}$ or right Cauchy-Green deformation tensor $\boldsymbol{C} = \boldsymbol{F}^T \cdot \boldsymbol{F}$, for instance. Its specific form is not of further interest at this point, but having in mind a simple hyperelastic material suffices. The interface energy can also have various formats and the following example introduces some of the most classic effects found for mechanical interfaces:

$$\psi_A = \gamma_0 \, \overline{\det}(\overline{\boldsymbol{F}}) + \psi_I(I_{\overline{C}}) + \psi_{II}(II_{\overline{C}}) + \psi_{\|}([\![\boldsymbol{u}]\!]) + k_1 \, \kappa + k_2 \, \kappa^2 + g_1 \, G.$$

The first part is linear in the determinant of the in-plane deformation gradient $\overline{\boldsymbol{F}}$. It specifically relates the energy to the relative change of interfacial area as $\overline{\det}(\overline{\boldsymbol{F}}) = \mathrm{d}a/\mathrm{d}A$. This term accounts for what is typically called surface tension in the context of capillary effects or the Young-Laplace equation. A typical result of the above first term can be a curved soap bubble, although neither the stress nor the energy depend on curvature. The linearity of the term simply dictates a reduction of interfacial area for $\gamma_0 > 0$ and additionally requires elastic bulk resistance for stabilization of the system; for example, in droplet formation. The prefactor of the in-plane Cauchy stress tensor, $\gamma_0 \, \overline{\boldsymbol{i}}$, becomes constant. It relates to the mere change in interfacial area and the respective difference between the energy potentials of neighbouring materials. Despite its common usage, the term surface tension can hence be misleading in some disciplines as it does not represent a stress in the classic sense of elasticity and can even be found by the name of surface energy. Moreover, the above definition relates to the undeformed configuration, while formulations in the deformed configuration simply employ the constant parameter ($\gamma_0 \, \overline{\det}(\overline{\boldsymbol{F}}) \, \mathrm{d}A \rightarrow \gamma_0 \, \mathrm{d}a$). A distinctive definition of interface energy, derived stress and elasticity is presented in Chapter 2, transferring the molecular description of a free copper surface to a continuum one.

The energy terms involving the interface invariants $\psi_I(I_{\overline{C}})$ and $\psi_{II}(II_{\overline{C}})$ represent typical strain-based, isotropic interface elasticity. The stretch of skin or inflatable components are examples that also reach non-linear elastic regimes. The interface stresses resemble the bulk-type stresses closely with respect to their format. A basic framework

is presented in Chapter 3 on sharp interfaces with and without coupling to the underlying bulk deformation. That chapter also extends the analysis towards anisotropy and out-of-plane contributions by considering displacement jumps, $\psi_{\parallel}(\llbracket \boldsymbol{u} \rrbracket)$, for example, to cover opening and closure of cohesive zones. Allowing for such imperfect interfaces with displacement or traction jumps also constitutes a basis for inelastic processes such as crack propagation.

The influence of mean curvature κ is well-established, for instance, for the bending of slender structures like plates, cloth or cells [8, 87]. At much smaller scales, the so-called Tolman length becomes influential by mean curvature of higher order when the atomistic energy potential depends on the curved shape of the interface. This is investigated in Chapter 6 for destruction-free ultrasound characterization of nucleating bubbles. Furthermore, the Gaussian curvature G, an intrinsic invariant, is quadratic in terms of the principal curvatures and its integral links to toplogy changes such as rupture or coalesence by the Gauss-Bonnet theorem. Crack propagation constitutes another application of the analysis of curved interfaces. Chapter 4 accordingly focuses on the soundness of curvature-dependent energies for damage evolution.

Just like bulk materials, of course, interfaces also show a vast variety in terms of inelastic material behavior. Viscosity can affect mechanical interfaces, for instance, in the form of lubricating films [111, 225] or structural damping in spacecraft structures [252]. A highly dissipative mechanism that is specifically relevant to contact interfaces is friction [32, 128], which can cause wear, damping and locking in materials and industrial systems. The utilization of interfacial energy and instabilities is illustrated in Chapter 5 by the examples of attenuating structures and topology optimization. The interfaces' shape can also be controlled by sintering processes [89, 138, 202], requiring a thermomechanical coupling [29, 80, 255].

Interface plasticity is another mechanism that can be assigned to interfaces and bulk phases alike [109, 185, 190]. This covers plasticity in soil liquefaction [76] as well as in metals accompanied by hardening and damage, e.g., at grain boundaries [68, 210]. Damage of interfaces can also incorporate debonding or near-surface cracking. This includes, for example, ductile fracture in cohesive zones [80] or damage mechanics with stiffness degradation by scaling of the elastic energy potential [174]. Chapter 4 will focus on the evolution of single cracks, while Chapter 6 eventually aims at exploiting the information interfaces and pores provide on a larger scale.

The above mentioned properties allow for numerous mechanisms that are special to mechanical systems with interfaces, for example, folding and buckling, scale effects, curvature interference, surface-bound waves, channeling of signals, microcrack evolution, debonding, shape optimization, information transfer and much more. Such features unique to mechanical interfaces motivated the following investigations. The overall reading, irrespective of the readers' potentially different backgrounds, shall shed light on the modeling, control and opportunities of mechanical interfaces in our various natural and artificial environments.

1.4 Gallery

The following gallery illustrates the diversity and richness of interfaces' roles in our environment before the detailed investigations begin. The natural and artificial systems are often depicted at different length scales with the largest magnifications showing a section down to approximately 1 mm diameter. Some of the pictures were also collected during the course of several lectures, serving as a motivation for new students and as an appreciation for the beauty of mechanical structures and materials.

Figure 1.1: Quartz crystal — Like in metals, interfaces do not only delimit distinct crystal orientations but can also exhibit twinning, where the compatibility of adjacent lattices allows for a finite intersecting region with shared lattice points [135, 152].

Figure 1.2: Grain boundaries of a pole — Grain boundaries play a vital role in manufacturing, for example, strengthening of steel via the Hall-Petch effect by pinning of dislocations [110, 196] or the formability of aluminum foil with many free grain surfaces [133, 149].

Figure 1.3: Ruhr sandstone — Understanding its microstructure is a key for risk assessment of construction work [12]. The interfacial area confining reservoir fluids can be in the order of 20 000 m^2/m^3 for the example of Bentheimer sandstone [125]. Inset shows the Steinerner Turm in Dortmund, Germany.

Figure 1.4: Banded standstone — The banded sandstone found in the Valley of Fire, Nevada, USA shows interfaces separating units of different color. Additionally, boundaries in the form of faults, compaction bands and changes of orientation are visible [62].

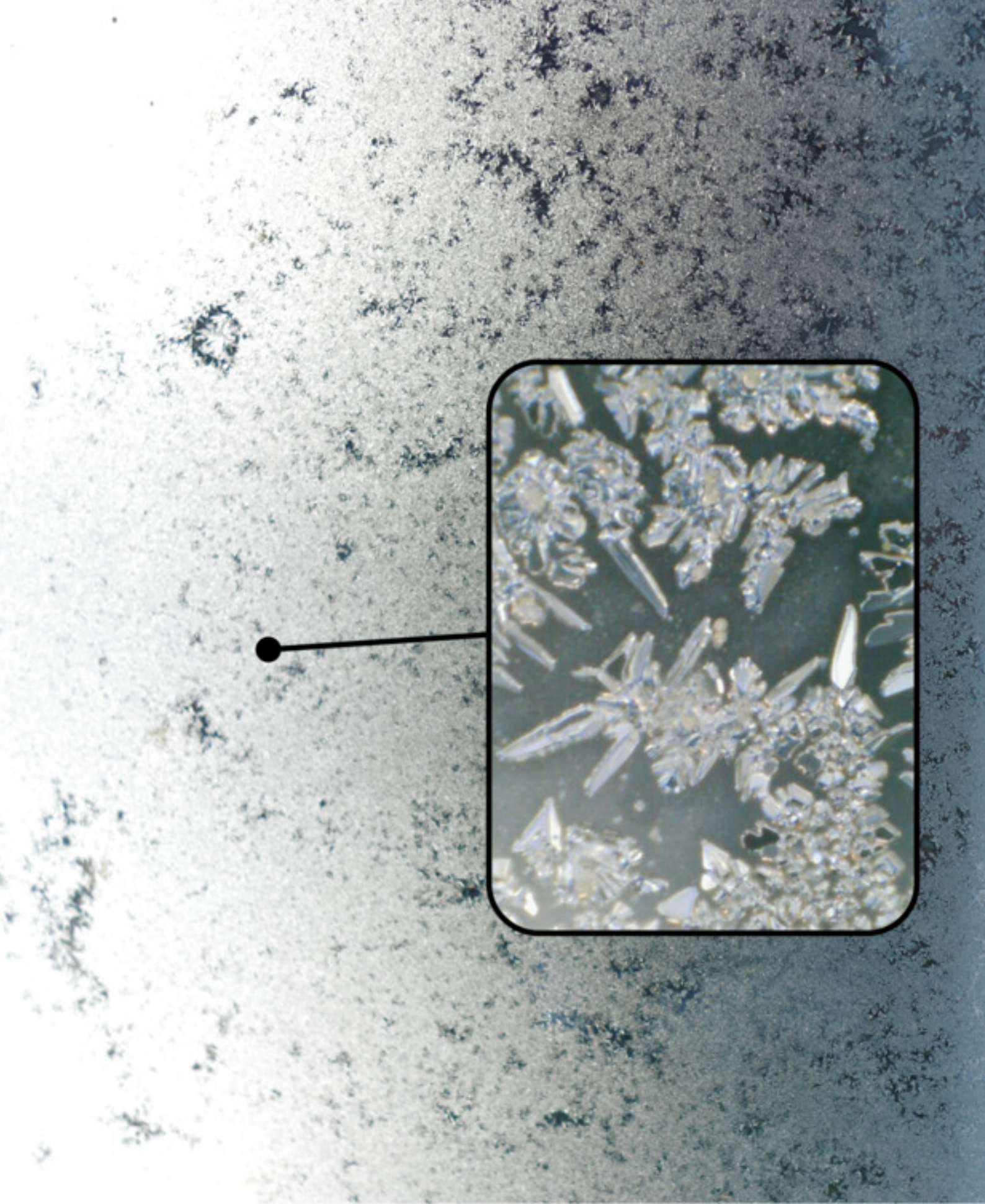

Figure 1.5: Frost crystals — Surfaces of frost crystals show an impressive abundance of geometric forms and grow with a fractal dimension of nearly 2 [157], which is almost twice as high as crack propagation in Ni-Cr steel [65]; both however depending strongly on ambient conditions.

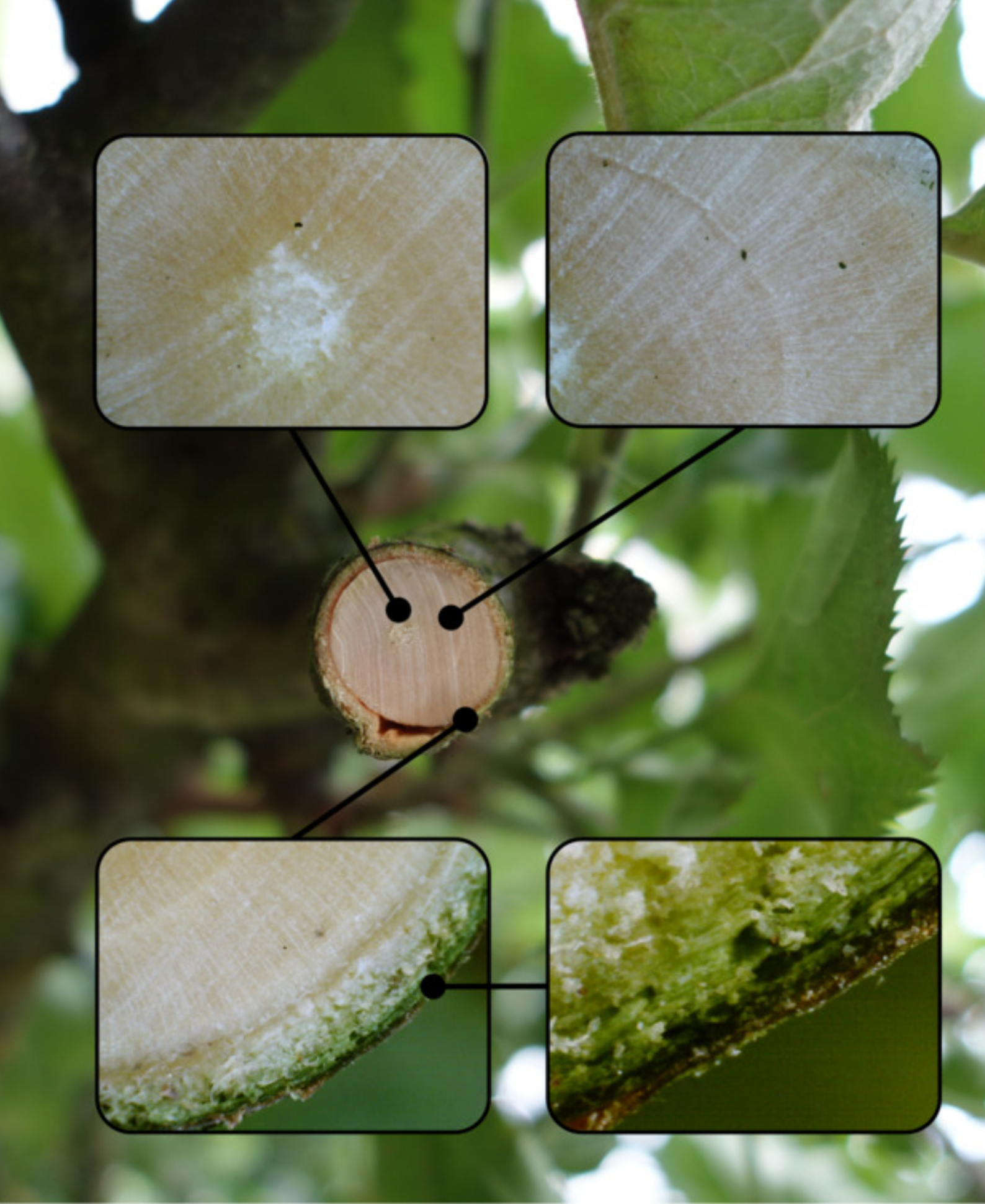

Figure 1.6: Branch of an apple tree — Interfaces of different orientation are visible from the inner pith to the outer bark and indicate a form that follows functions such as nutrient transport, stability and protection in plant growth [214, 237].

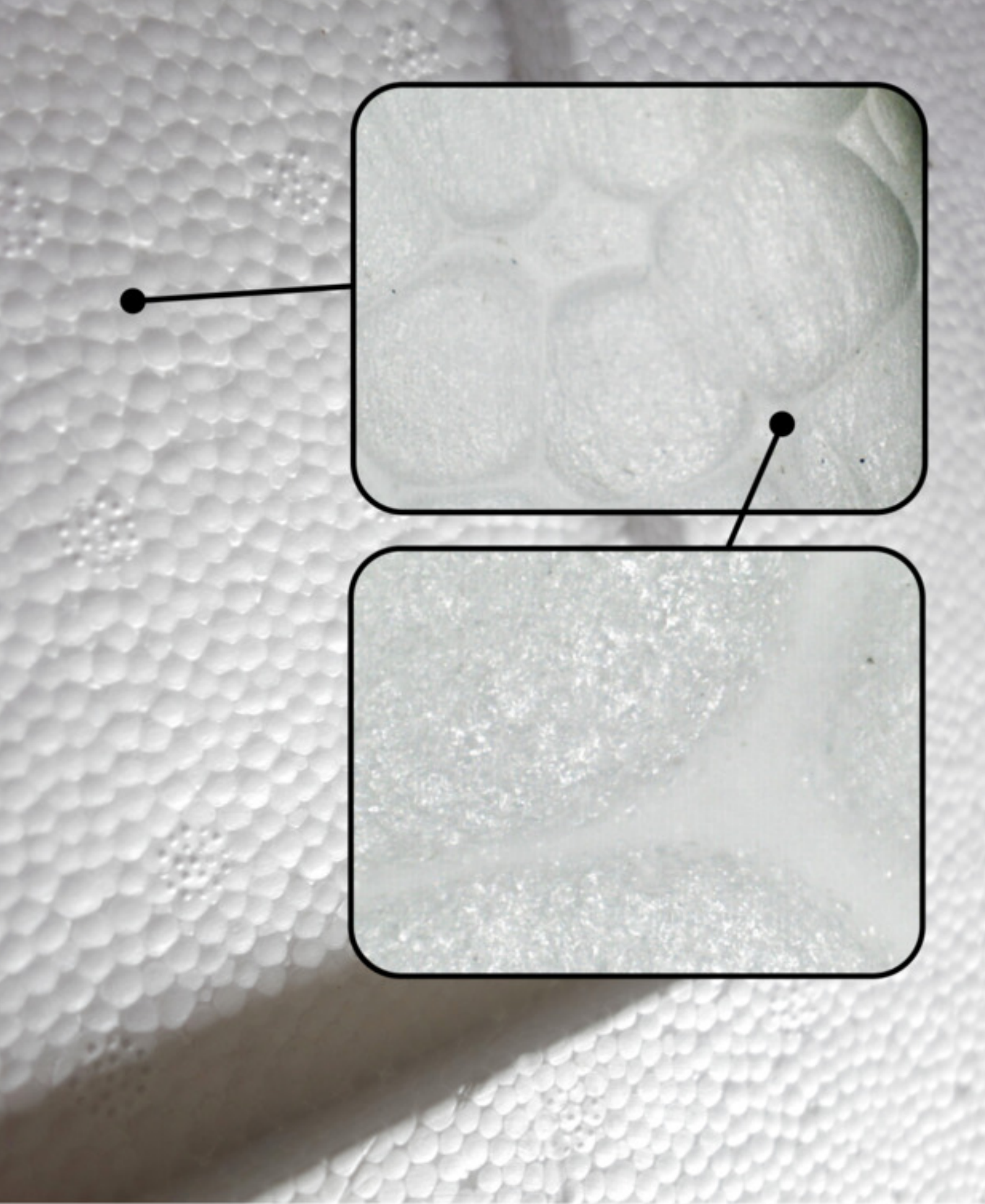

Figure 1.7: Expanded polystyrene — The cell structure of expanded polystyrene allows for significantly low thermal conductivity and light weight, e.g., $0.04\,\mathrm{W/(m\,K)}$ for a density of $52\,\mathrm{kg/m^3}$ and a mean cell size of $632\,\mu\mathrm{m}$ [1].

Figure 1.8: Shaving cream — Surface tension allows foams to sustain a stable shape for long periods of time. Their application ranges from lubrication and transport of enclosed particles in health care to conditioning agents for cohensionless soils supporting excavated grounds [258].

Figure 1.9: Shear band in a sand column — While frictional grain-grain interfaces determine the angle of repose of dry sand surfaces (34°), the high energy of water-air interfaces stabilize wet sand (45°, similar to shredded coconut) [19, 94]. Shear bands can form due to a macroscopic loss of stability [25].

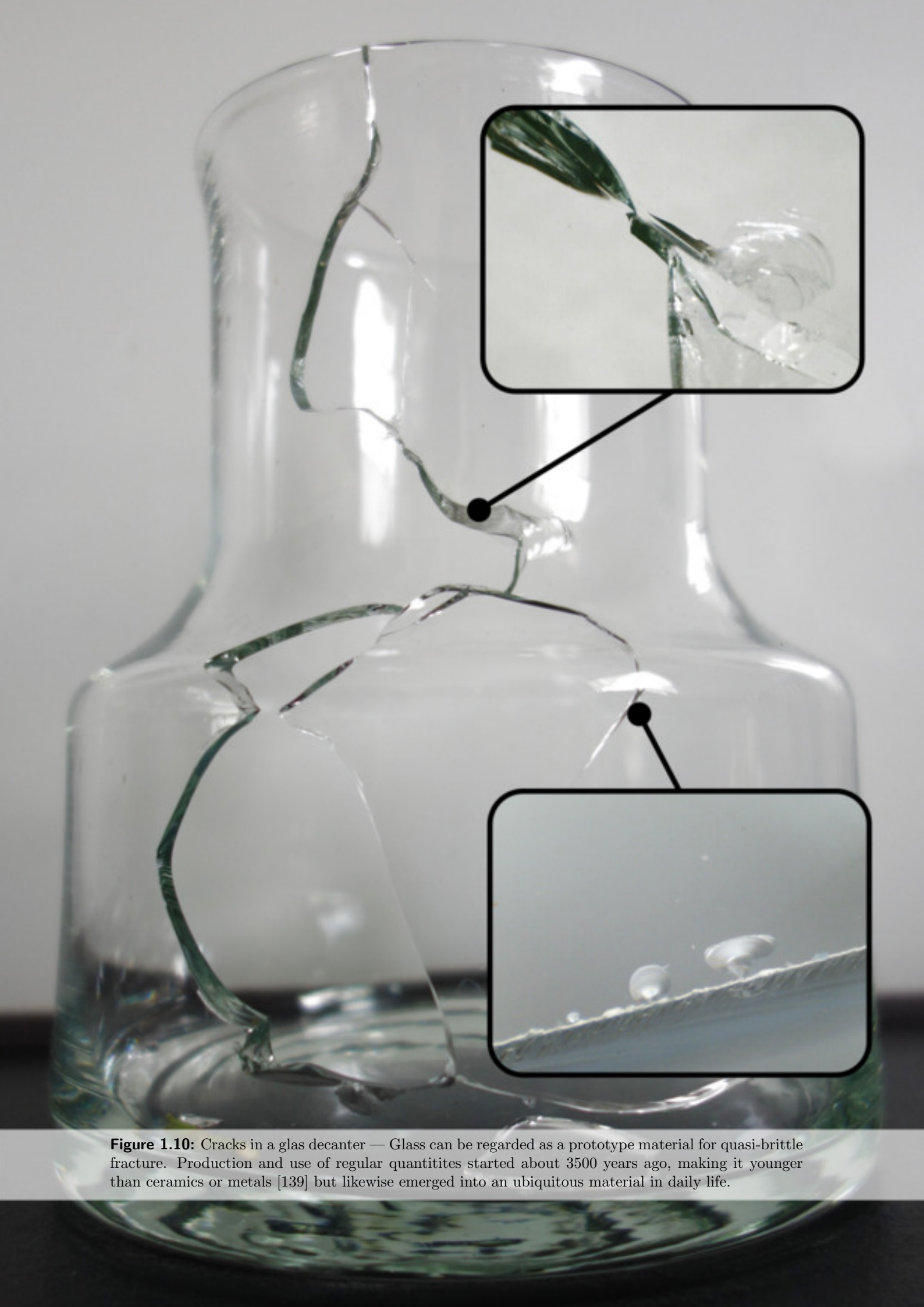

Figure 1.10: Cracks in a glas decanter — Glass can be regarded as a prototype material for quasi-brittle fracture. Production and use of regular quantitites started about 3500 years ago, making it younger than ceramics or metals [139] but likewise emerged into an ubiquitous material in daily life.

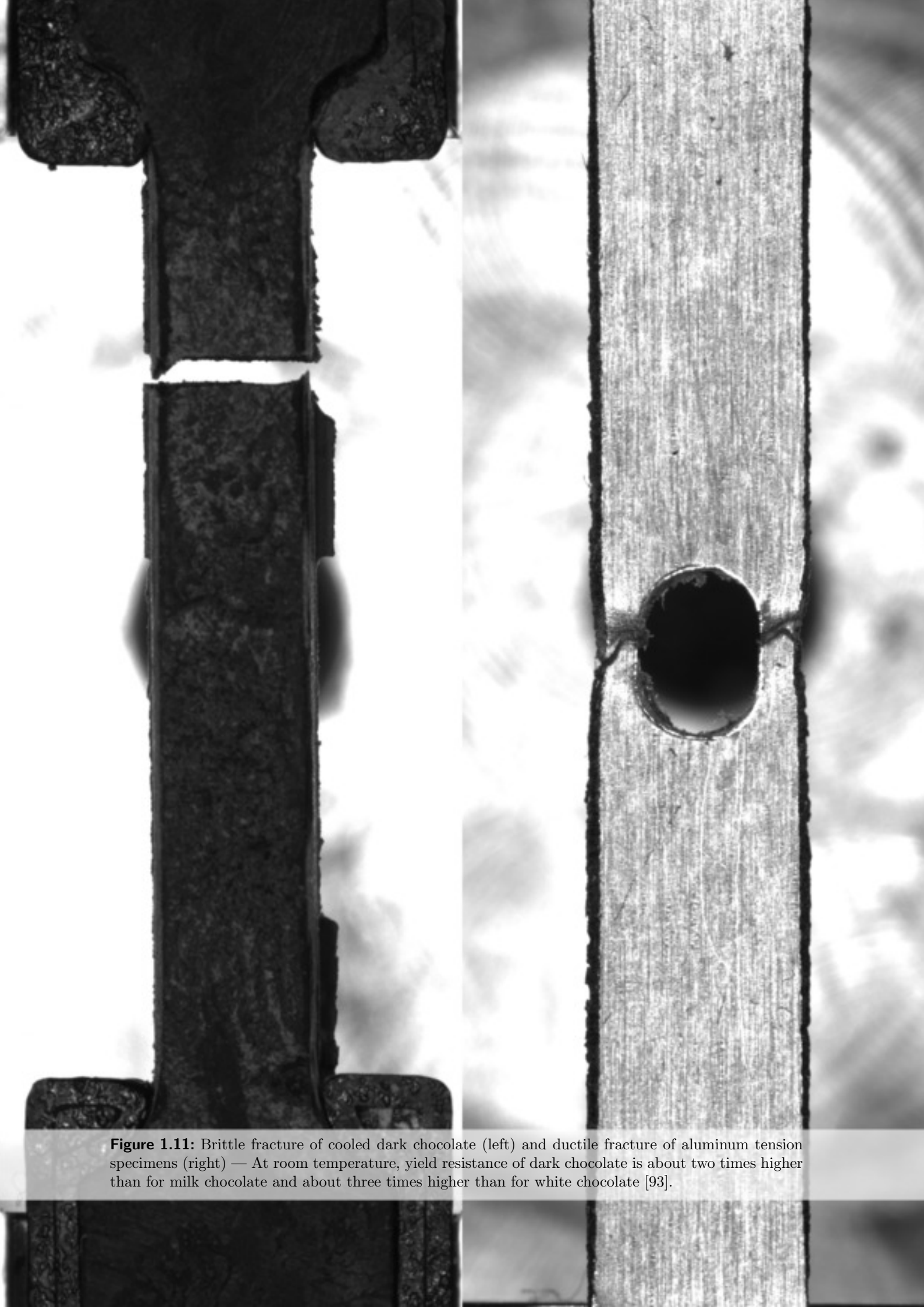

Figure 1.11: Brittle fracture of cooled dark chocolate (left) and ductile fracture of aluminum tension specimens (right) — At room temperature, yield resistance of dark chocolate is about two times higher than for milk chocolate and about three times higher than for white chocolate [93].

Figure 1.12: Brittle fracture of a steel ice hockey blade (left) and ductile fracture of a case-hardening steel specimen (right) — The associated elastic and plastic deformations, respectively, cause the characteristic fracture surfaces [195].

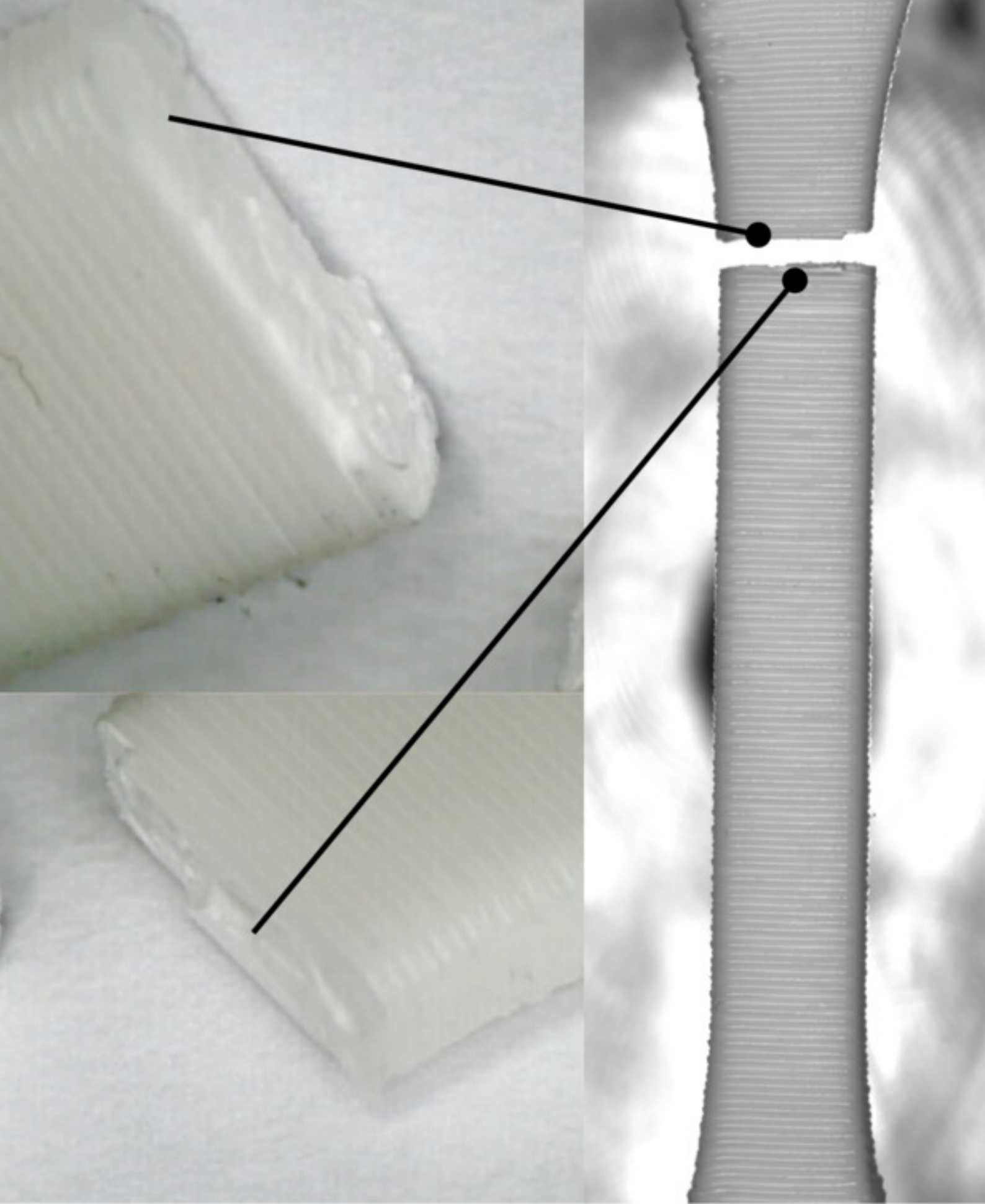

Figure 1.13: Cracks in 3d-printed polyactiv acid (PLA) — Cracking of PLA in 3d prints via fused deposition modeling (FDM) depends strongly on the orientation of the layers. The fracture load is almost half for 90°specimens compared to 0°specimens [141].

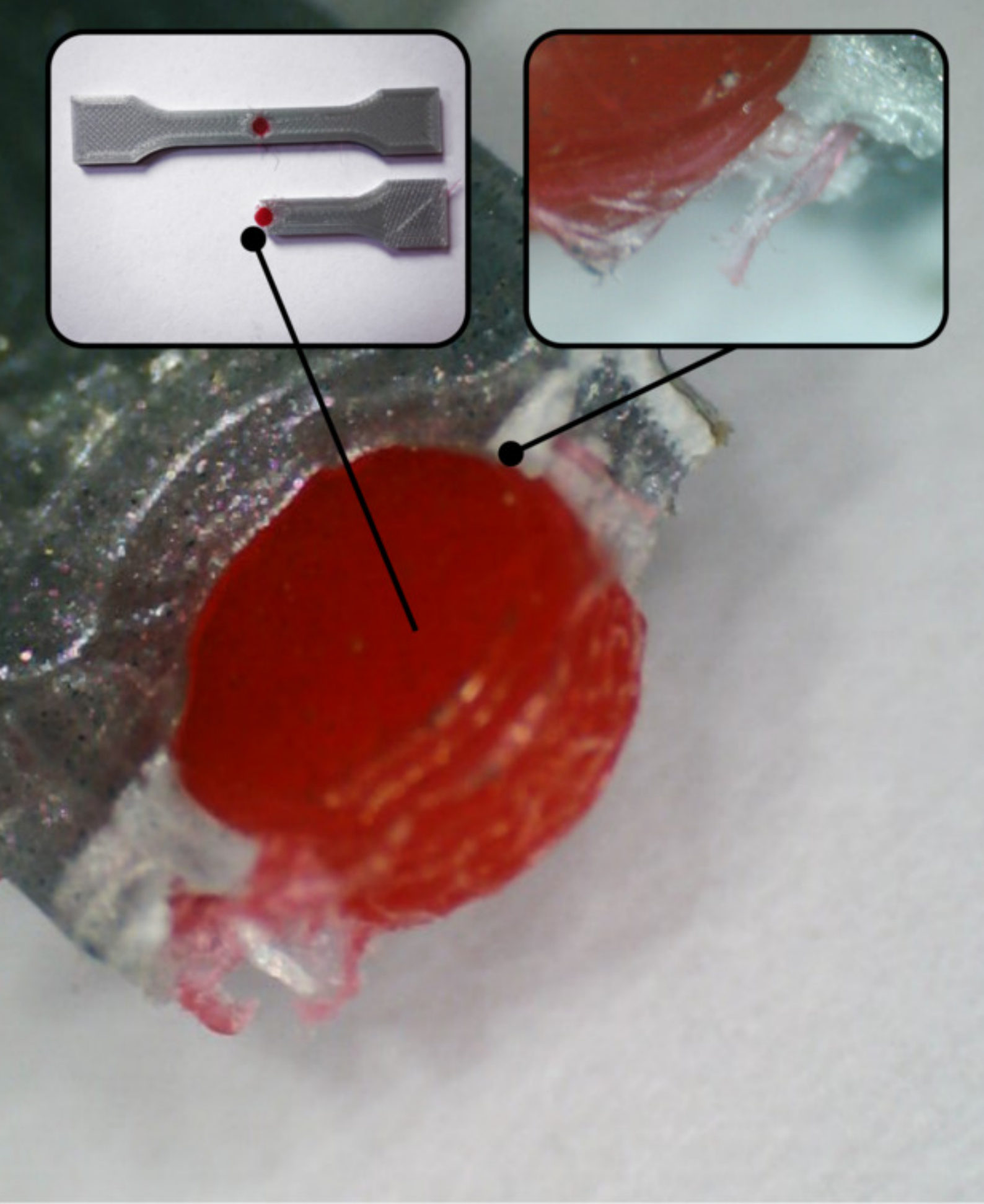

Figure 1.14: Cracked 3d-printed polyactiv acid (PLA) tension specimen with thermoplastic polyurethane (TPU) inclusion — Remnant fibres indicate a non-trivial detachment, which is why the interfaces play an important role in reinforced structures [96, 230].

Figure 1.15: Disc brake of a car — Due to friction when slowing down vehicles, the temperature of disc brakes can increase by a few hundred degrees, e.g., reaching 800°C after four repetitive short-term brakes [256].

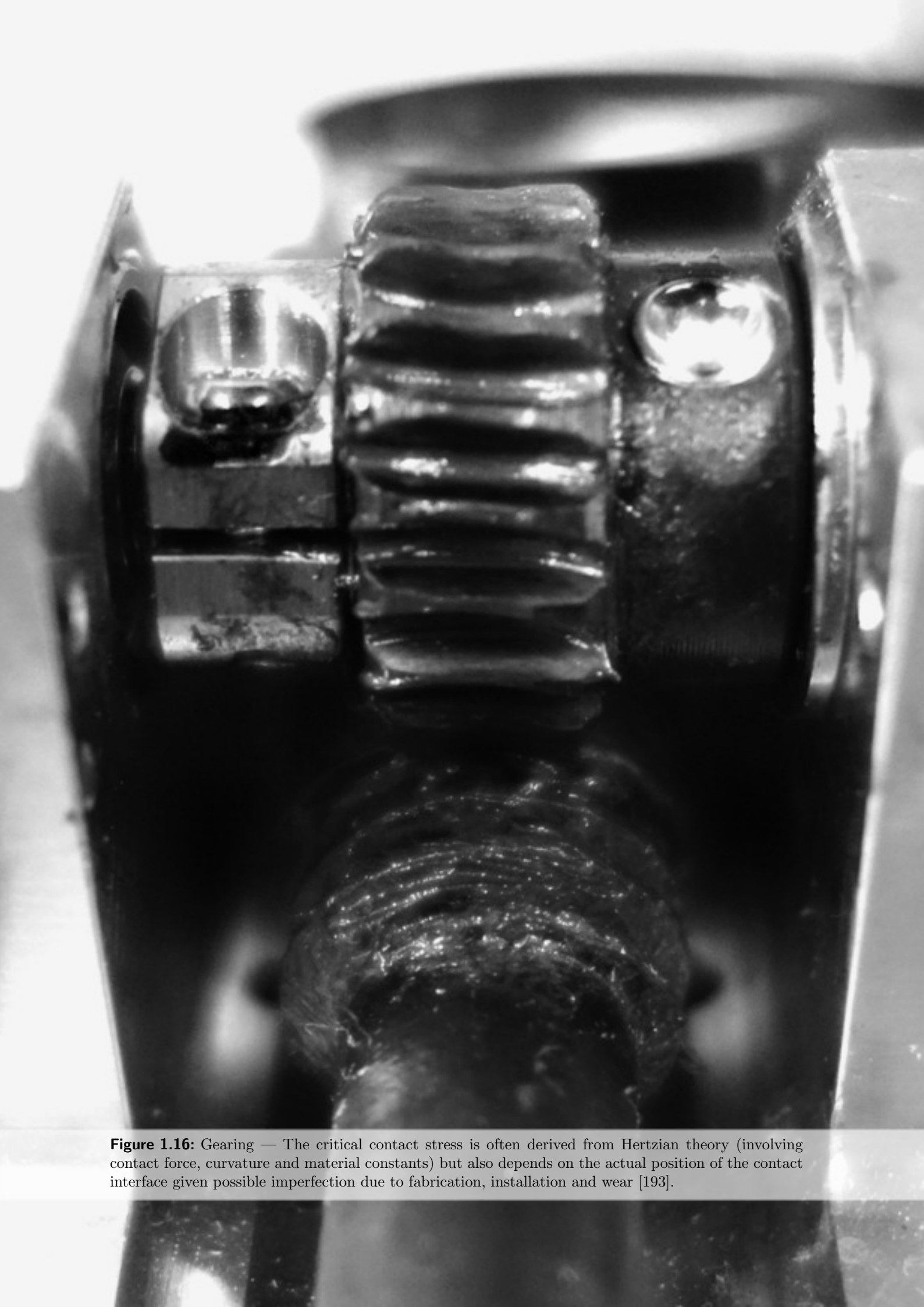

Figure 1.16: Gearing — The critical contact stress is often derived from Hertzian theory (involving contact force, curvature and material constants) but also depends on the actual position of the contact interface given possible imperfection due to fabrication, installation and wear [193].

Figure 1.17: Welding seam — Welding creates a joining area of contact that contains the fusion line itself (where the material is melted) but also a heat-affected zone (where the material does not melt). Alteration of the latter microstructure can cause risks in the form of reduced tensile strengths. [129]

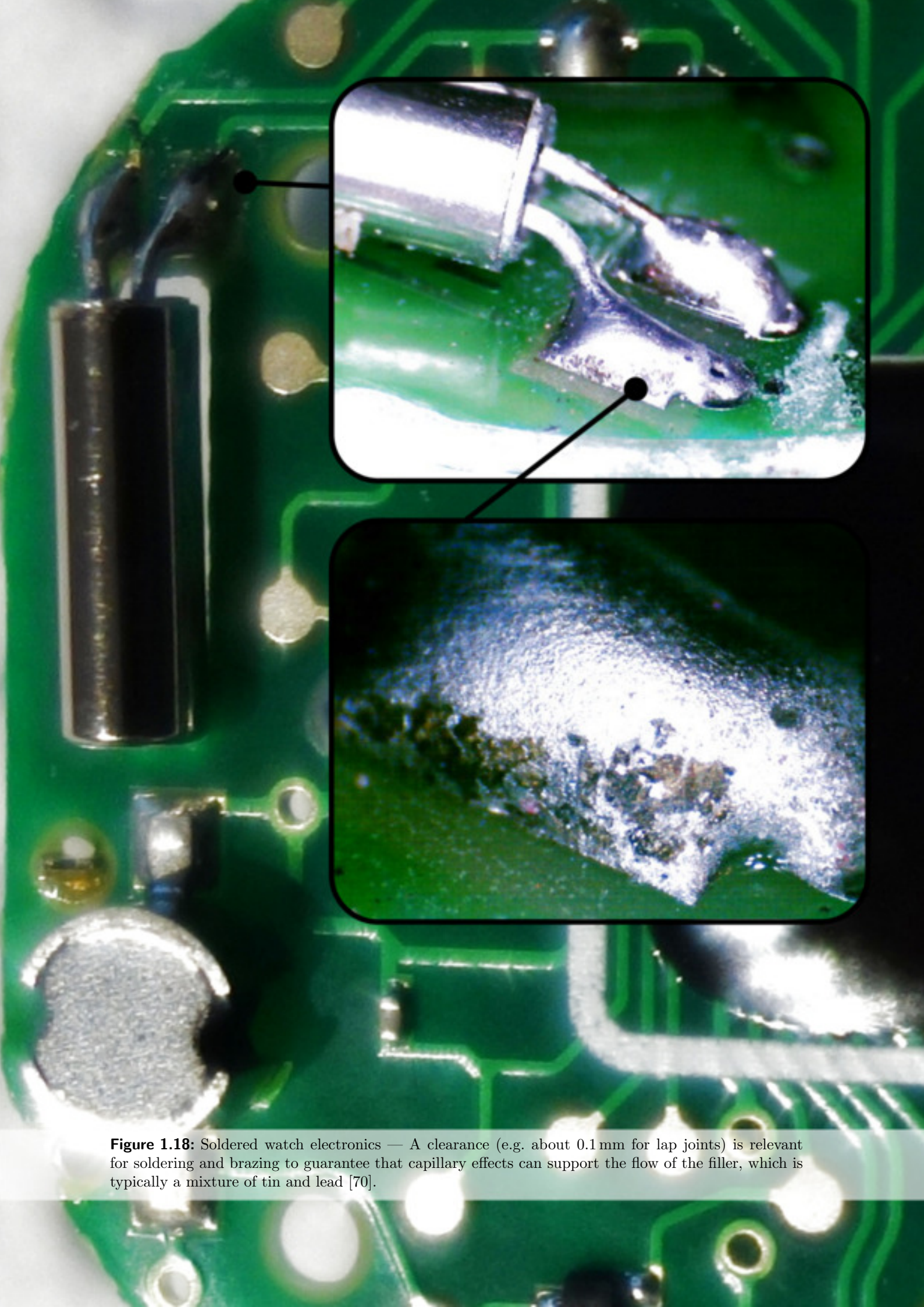

Figure 1.18: Soldered watch electronics — A clearance (e.g. about 0.1 mm for lap joints) is relevant for soldering and brazing to guarantee that capillary effects can support the flow of the filler, which is typically a mixture of tin and lead [70].

Figure 1.19: Coin — The 1 € coin is composed of an inner copper-nickel circle and an outer nickel brass ring. Over eight billion 1 € coins circulated as of 2022, which is 5.6 % of all € coins by quantity or 24.8 % by value [78].

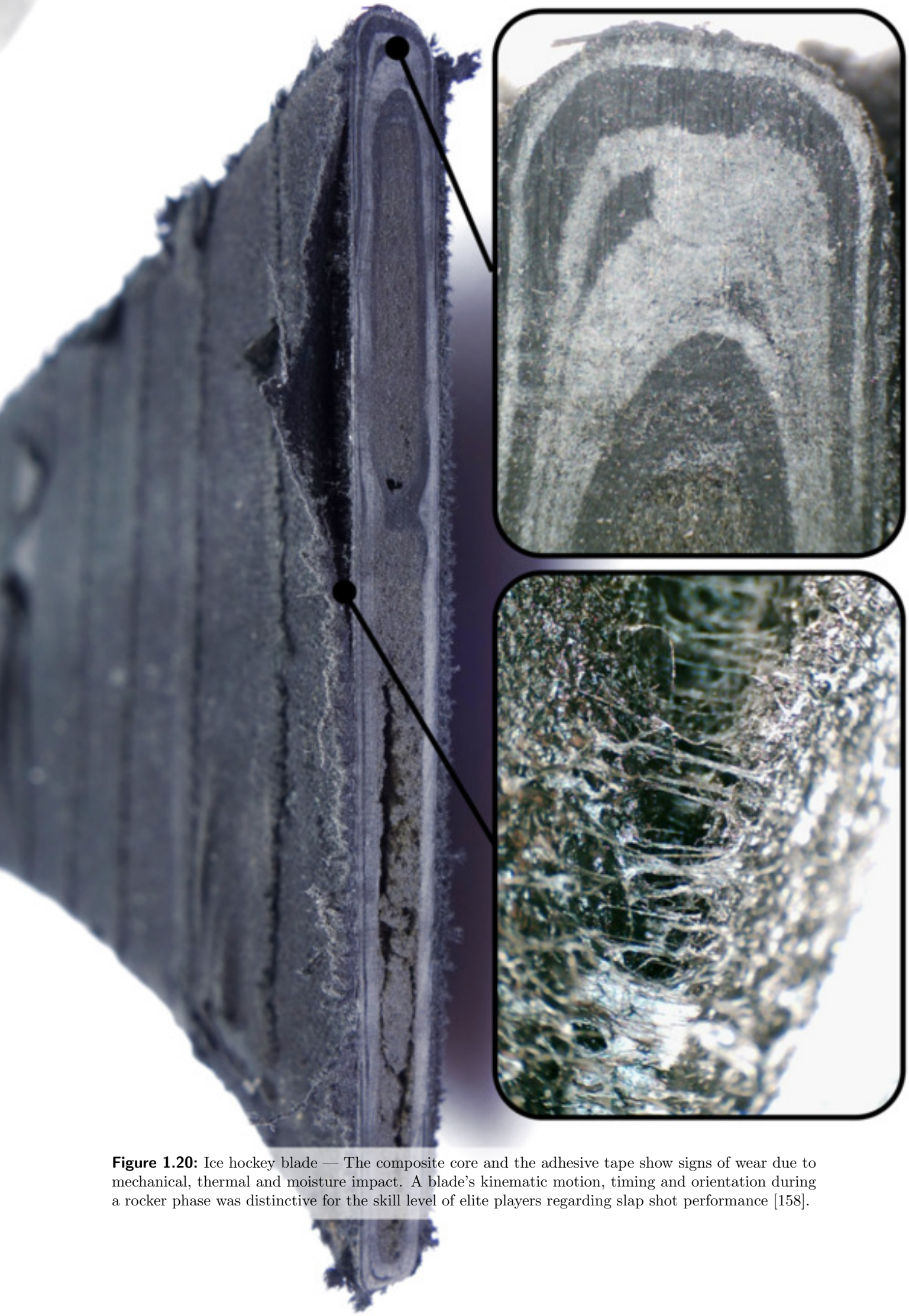

Figure 1.20: Ice hockey blade — The composite core and the adhesive tape show signs of wear due to mechanical, thermal and moisture impact. A blade's kinematic motion, timing and orientation during a rocker phase was distinctive for the skill level of elite players regarding slap shot performance [158].

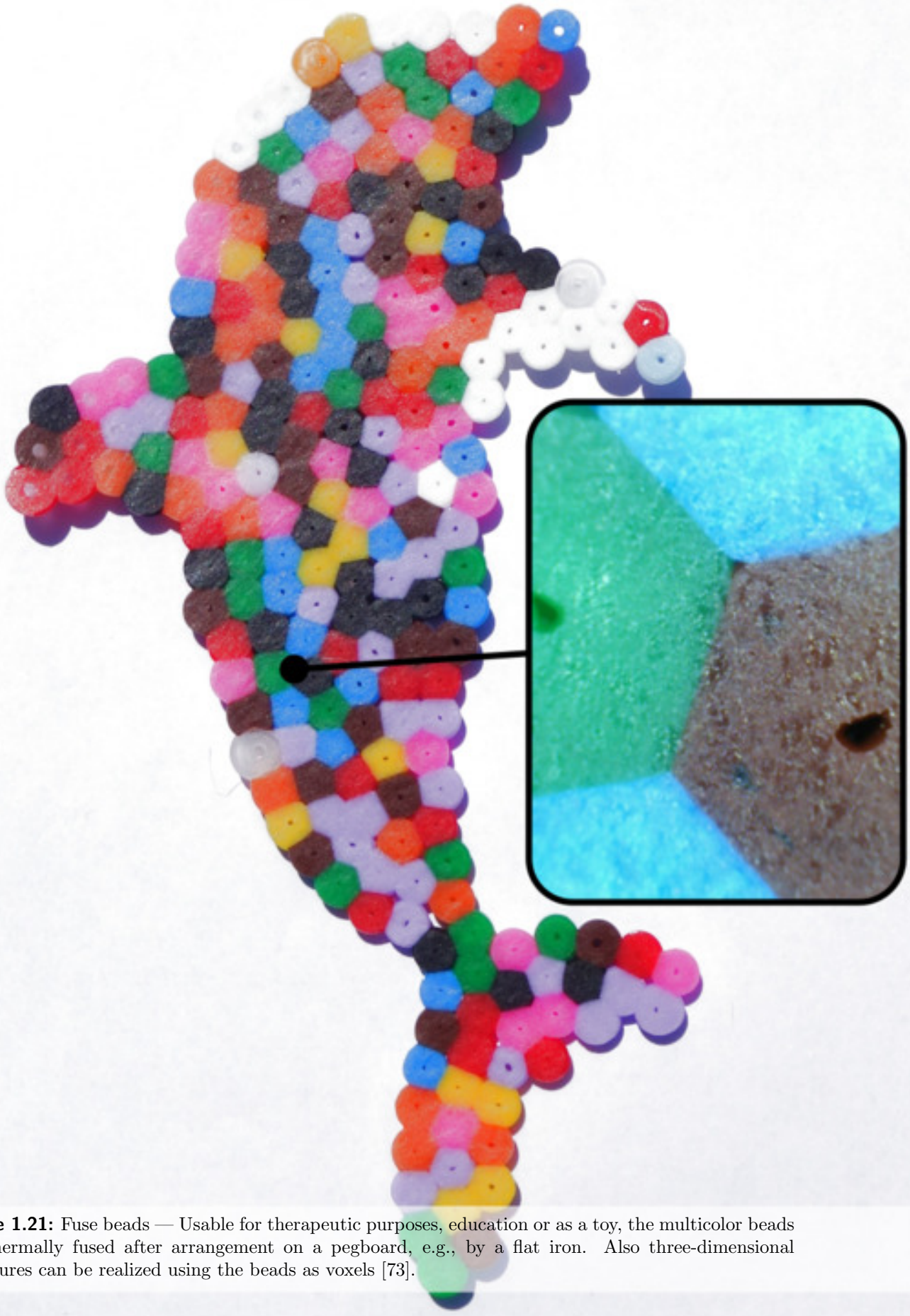

Figure 1.21: Fuse beads — Usable for therapeutic purposes, education or as a toy, the multicolor beads are thermally fused after arrangement on a pegboard, e.g., by a flat iron. Also three-dimensional structures can be realized using the beads as voxels [73].

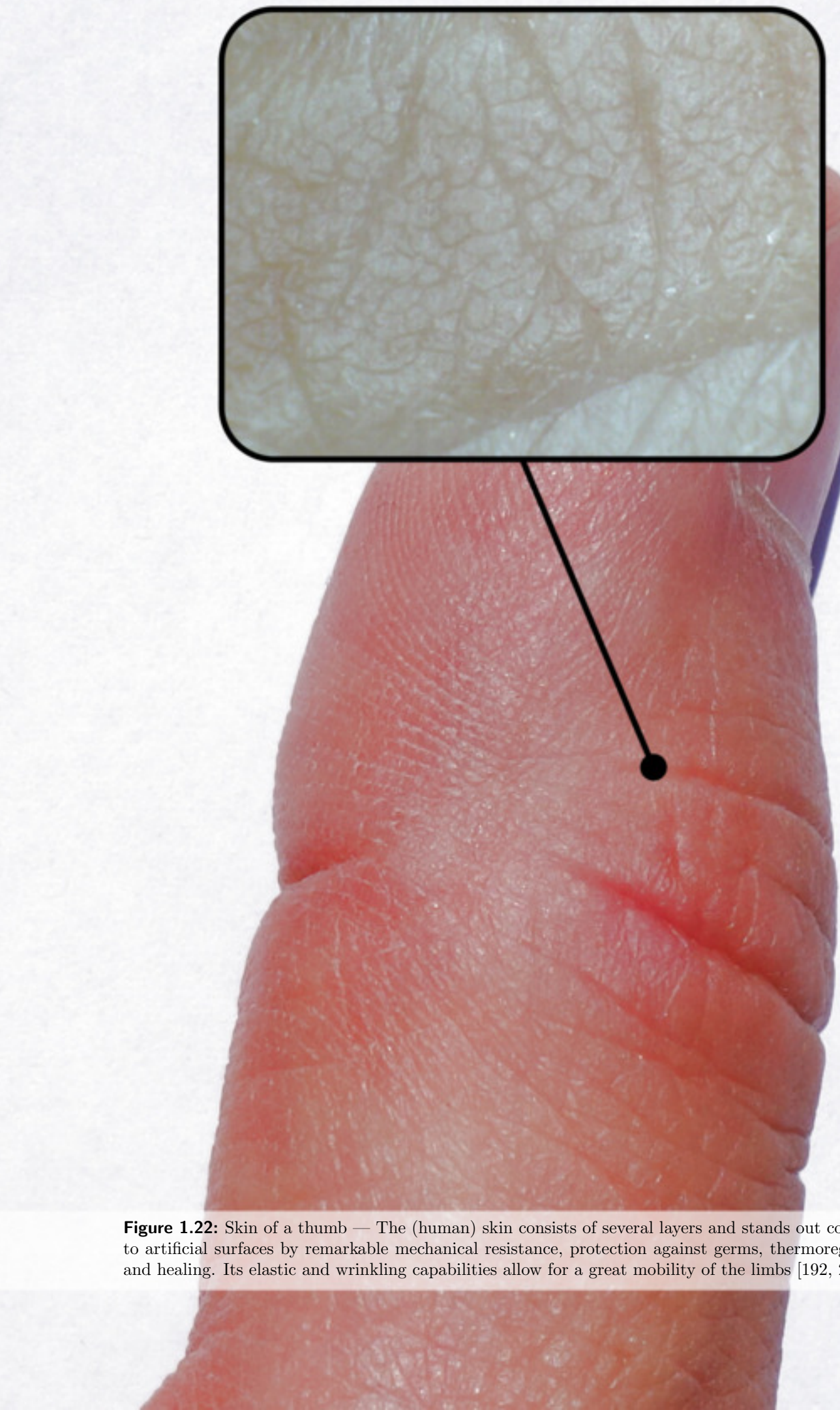

Figure 1.22: Skin of a thumb — The (human) skin consists of several layers and stands out compared to artificial surfaces by remarkable mechanical resistance, protection against germs, thermoregulation and healing. Its elastic and wrinkling capabilities allow for a great mobility of the limbs [192, 249].

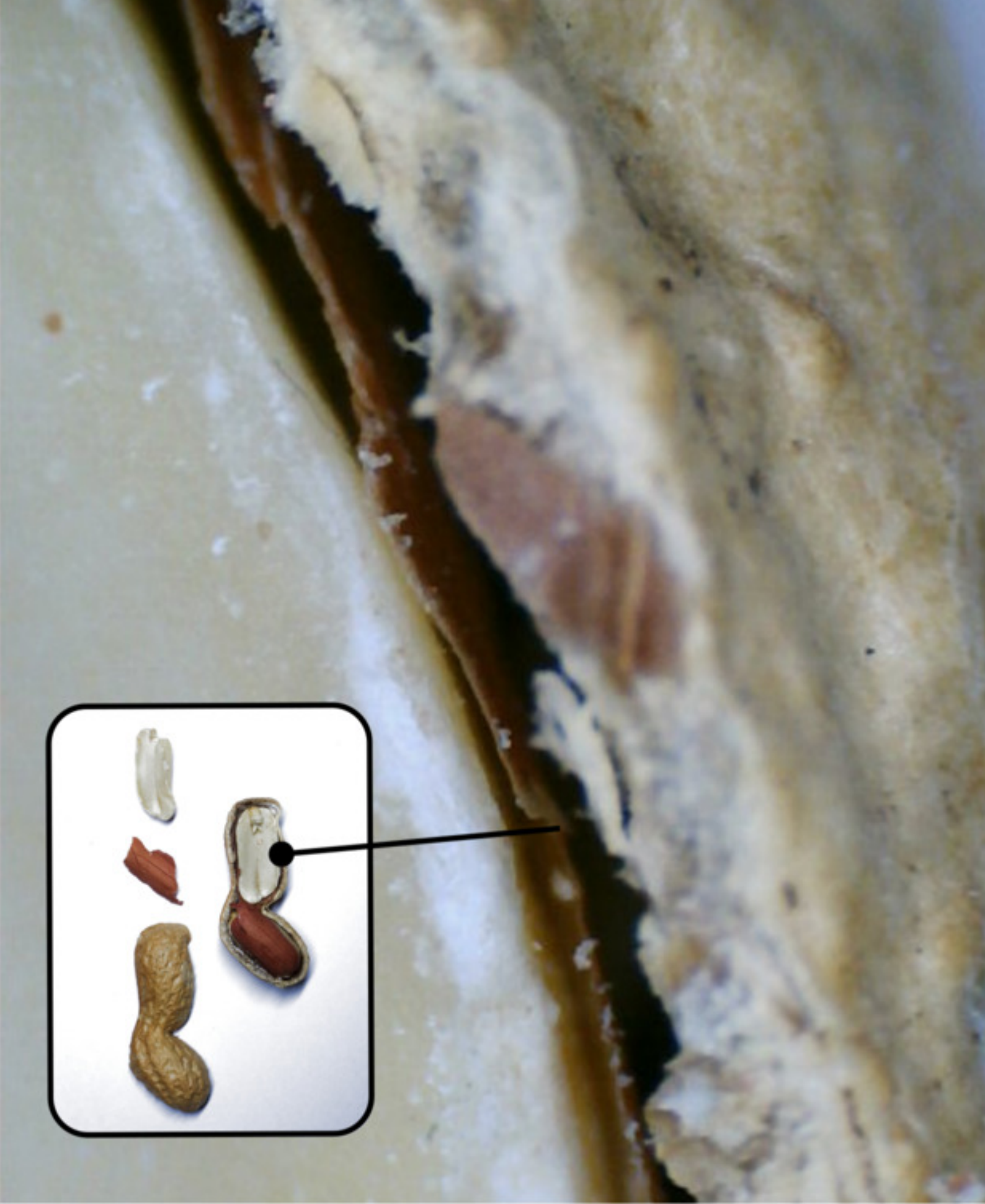

Figure 1.23: Peanut — Peanut fruits can withstand rupture forces up to about 100 N but less when moist or reduced to their kernel [10]. Knowing their fatigue behavior helps to optimize shelling conditions in automated production such as friction and applied forces [108].

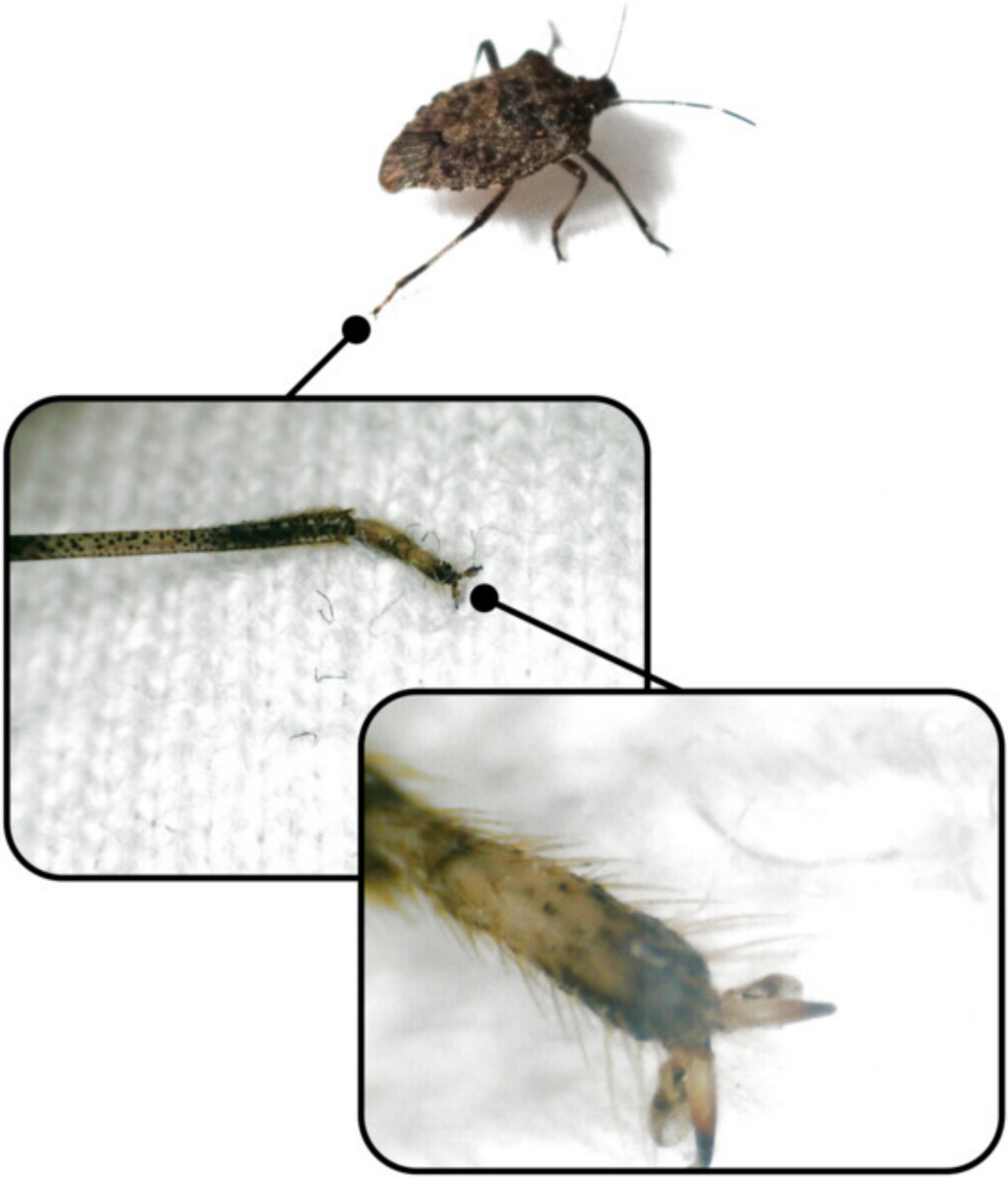

Figure 1.24: Contact zone of bug leg on fabric — Many insects can climb even vertical surfaces thanks to fine adhesive hairs at fibrillar foot pads [41] and also pad secretion was shown to act as a possible support for the adhesive pads [144].

Figure 1.25: Snail climbing a vertical wall — Snails can produce mucus on which they move with their muscular foot. Locomotion is achieved by muscular waves for many gastropods and supported by a yield of the mucus at larger strains, recovering for the next wave of forward motion [63].

Figure 1.26: Water-air and sand-water wavy interfaces — Wind waves can be used to verify information on the characteristics of seas on earth and other objects of the solar system [159]. Ripple formation at the ground tells whether the particles' Reynolds and Froude numbers stabilized deposition [33].

Figure 1.27: Water drops — Water drop formation is one of the easiest possibilities to observe the impact of surface energy with the naked eye. The interface energy of 70 mN/m for water and air is among the highest of natural interfaces [58].

Figure 1.28: Paving joints compensating elastic and plastic deformation — besides their mechanical properties [160], interface regions can serve various other puroposes such as hydraulic conduits, filters or even ruderal microhabitats.

2 From atomistic to continuum desription of interfaces

2.1 Introduction: Atomistic and other underlying origins of interfaces and their homogenization

Many interface effects are well-known to appear on length scales smaller than observable by the human eye. One purely geometric reason is that the ratio of interfacial area to bulk volume increases with smaller size. For instance, grain boundary and dislocation evolution [39, 68, 203], curvature phenomena [238] and crack initiation are typically sub-mm processes [228]. Materials with a significant amount of inherent interfaces hence strengthen interface-related mechanisms. This can be achieved, for example, by higher porosity, creases or finer structures, such as the thermal insulation of light-weight aerogels [145] or the susceptibility to crack propagation in fine-grained copper [195]. Also non-mechanical properties such as the efficiency of chemical and electrical processes rely on smaller scales [167].

Another motivation for approaching interfaces from a smaller length scale is the classic bottom-up approach in multi-scale physics. This means driving the understanding and description of interface physics by understanding the underlying processes. The formation of interfaces can often be traced back to the difference of the atomistic energy potential between the two neighboring bulk materials, causing a rearrangement of the atoms' positions near the interface. Localized changes of volume, density, stress or energy accordingly motivate the assignment of such (excess) properties to an interface model [75, 253]. This includes phenomena like interface-dominated diffusion during sintering [89, 138] or plasticity and damage on the atomistic scale [210]. The view on smaller scales also challenges the validity of assumptions like zero-thickness interfaces or in-plane stresses, e.g., see the Gibbsian description accounting for finite width and rigorous thermodynamic treatment in [182]. Respective models relate to first-principles, e.g., in fields like quantum chemistry, density-functional-theory, kinetic Monte Carlo or molecular dynamics simulations. The subsequent Section 2.2 lays a focus on the formation of interfaces on the atomistic scale with the example of copper by using molecular dynamics simulations.

While atomistic descriptions can allow an insight into detailed interface mechanisms, continuum descriptions can allow for an efficient, effective description. Having both at hand, yet, does not provide a complete picture without connecting them. This can be achieved by homogenization techniques. The many-sided facets of homogenization

yielded numerous implementations, e.g., see [53] for a broad but concise overview. Distinctions of available homogenization approaches can be made between deterministic and stochastic, random and periodic, and many more classifications. The simplest homogenization concept may be regarded to be spatial averaging over representative volume or interface elements. In any case, a careful interpretation of homgenized properties is necessary. On the one hand, for example, stresses may be derived from the basis of an energy potential and an energetically dual, homogenized strain. On the other hand, stresses may be derived from a time- or space-averaged (ergodic) momentum flux of atoms across boundaries. Such ambiguity bears the challenge of a consistent split into mechanical and thermal contributions, because variables such as temperature are not a-priori defined on the atomistic scale.

Two concepts relating to homogenization should deserve explicit mentioning, upscaling and coarse graining. A unique definition among all disciplines is again difficult to find. Upscaling methods typically depend on scale separation, e.g., different length scales of the atomistic and continuum descriptions. This can be a beneficial assumption that allows relaxing simplifications, because effects on smaller and larger scales may become negligible. One famous illustration of this concept is simple volume averaging to obtain volumetric ratios or densities. It often employs the idea of representative volume elements (RVEs), cf. Fig. 2.1. Scale separation is not a strict requirement for homogenization in general, though. To be mentioned at this point is that further length and even time scales can be involved for interface mechanics. For example, continuum-to-continuum approaches instead of atomistic-to-continuum transitions are often sufficient to approach processes on the geophysical scale [85] such as the formation of faults inside the earth's crust [166, 177]. The discussion of systems on larger length scales with multiple internal interfaces and the homogenization thereof will also be continued in Chapter 5 and Chapter 6. Moreover, time scales are relevant in order to derive effective interface models, e.g., grain-boundary evolution during creep [195] or the viscoelastic response of the lithosphere [142].

The other term to be mentioned explicitly is coarse graining. It can often be found in the combination with complex stochastic systems, which is not limited to atomistic systems. It can also cover granular media, for instance [204]. The QuasiContinuum Method is a coarse-graining method that captures the atomistic-to-continuum transition within a finite-element framework [233, 234]. It connects atomistic and continuum physics by the incorporation of interatomic interactions into a finite-element analysis through a crystal calculation based on the local state of deformation. A possibly associated energy minimization will be replaced by a constrained energy minimization over a subset of representative atoms. This also allows the investigation of interface effects inside crystals and at their boundaries [222], which are particularly relevant at the smaller length scales.

Another coarse graining particle-to-continuum approach can be realized, for example, by a multi-particle collision dynamics (MPC) framework. Even though MPC can be used for atomistic simulations, it can also cover thermal fluctuations based on stochastic

dynamics of larger particles. This allows finite-size simulations from the mm-scale to the m-scale. Particle-particle interactions then do not necessarily resemble atomistic behavior but are also set up, for instance, to effectively mimic Navier-Stokes fluids or microswimmers therein. They can reach a sweet spot between classic continuum descriptions that do not consider underlying fluctuation fields and atomistic descriptions that would exceed the available computational resources for larger systems.

The following investigation in Section 2.2 will illustrate the link between an atomistic and a continuum interface description of copper by a Ritz-type computational homogenization. In accordance with the Hill-Mandel condition, the idea of energy equivalence is taken up to derive continuum properties from the atomistic simulations. The subsequent study in Section 2.3 uses an MPC-based framework, MP^{2}C, which shows a significant scalability potential on hundreds to thousands of computational cores. Its application will be demonstrated by the example of suspensions in annular shear flow with interfaces governing the particle-wall, fluid-wall and fluid-particle contact.

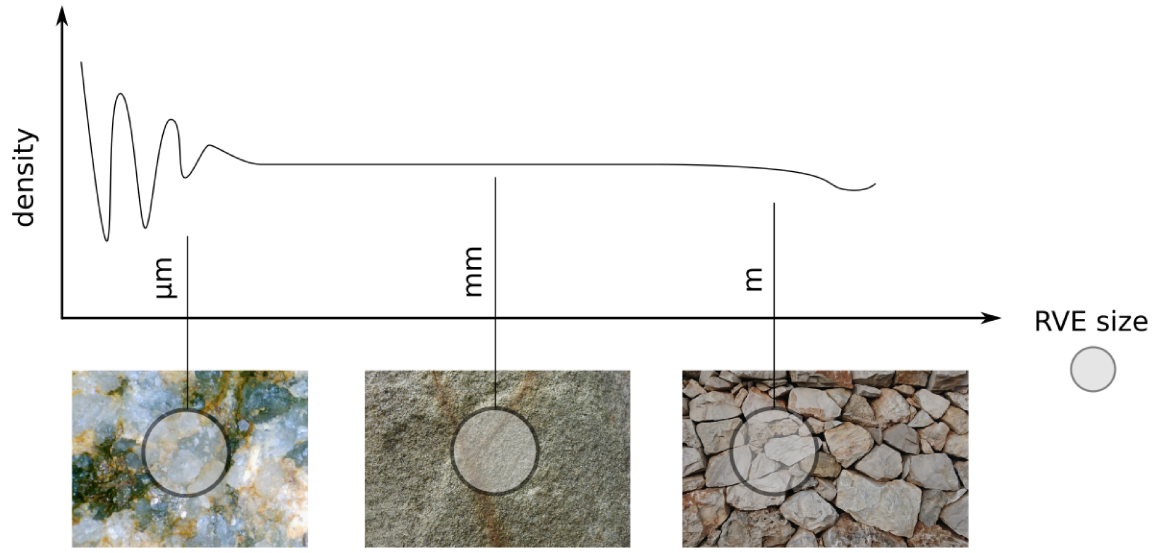

Figure 2.1: Sketch of the RVE (Representative Volume Element) concept for a volume-averaged density. The middle length-scale interval is not affected by the RVE size and thus suitable for a homogenized definition of density. Lower and upper limits appear, where scale separation between the RVE size and the systems's structure no longer holds.

2.2 Computational homogenization of material surfaces: From atomistic simulations to continuum models

Scale effects are relevant for both interface analysis and design because the interface-to-volume ratio changes with the length scale of the system. Often, interesting effects such as interface-induced stiffening, curvature interference or phase changes are conceptually

discovered. However, the quantitative impact on practical systems, for better or for worse, remains to be clarified. Despite the abundance of investigations, a comprehensive set of material parameters for continuum interface models is still rare. A possible difficulty is the separation of some effects between the molecular and the continuum level.

The following study provides a framework to derive continuum surface properties from atomistic simulations by a Ritz-type computational homogenization. The key idea is the coupling of atomistic and continuum representative volume elements with free surfaces. The energy equivalence under various loading conditions yields the elastic surface parameters by the example of copper, see Fig. 2.2 for an illustration of the idea. The results moreover reveal that the creation of a free surface induces a zone of a few atomistic layers that show rearrangement of the atoms' positions and a change of the energetic landscape. This implies that the systems of investigation must allow for a minimum system size for full evaluation of the surface domain.

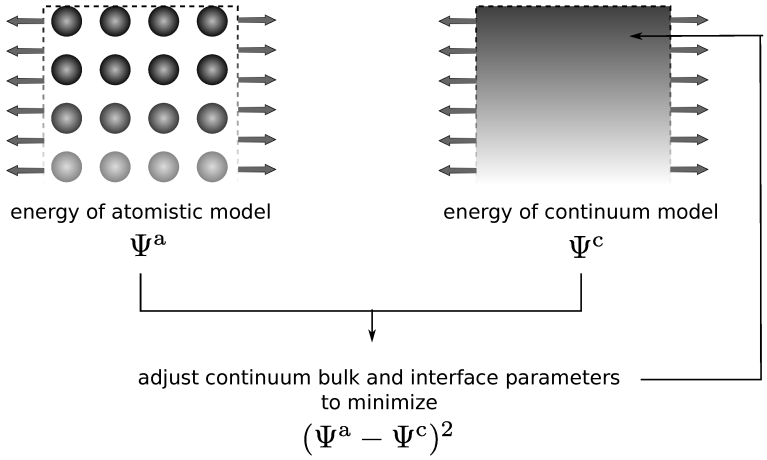

Figure 2.2: Ritz-type homogenization of bulk and interface by adjusting their continuum parameters for minimization of the energy difference between the atomistic and the continuum model.

Another crucial outcome is that the idea of assigning excess properties to an interface via the concept

$$\text{interface} = \text{total system} - \text{bulk}$$

is not trivial. Indeed, using continuum bulk and interface models inevitably induces modeling errors as models are an approximative compromise between accuracy and practicability. The bulk error, however, will propagate to the interface model and induce a bias to it. Reducing this bias is possible by reducing the bulk phase. This goal contradicts the aim to allow for a fully developed surface region. The specimen of investigation must be small to reduce the bulk error, but also large enough to allow for fully developed surfaces. A physically sound definition of limits is thus required for the determination of interface or surface properties as will be shown in the following investigation.

Designated publication note

The treatise continues with the following publication(s) as a selected in-depth investigation for the present chapter (it can be found in the concluding chapter of scientific contributions, but may be excluded in public versions for copyright reasons):

C. Sievers, J. Mosler, L. Brendel and P. Kurzeja. Computational homogenization of material surfaces: From atomistic simulations to continuum models. *Computational Materials Science*, 175: 109431, 2020. doi:10.1016/j.commatsci.2019.109431.

2.3 Stochastic particle-based fluid-structure interfaces in suspensions in annular shear flow under gravity: simulation and experiment

Just as interface effects are known to become more dominant on smaller length scales, so can thermal fluctuations. Diffusion and suspensions are two examples, of which the latter will serve as an example in the following study. The Brownian motion of small particles is of relevance in many technical and biomedical fields. Microswimmers, for instance, attracted recent interest as a special tool for drug sensing and delivery. Biological microswimmers at the µm-scale such as bacteria and sperm motivated the development of synthetic counterparts like Janus particles with two different coatings. Also filtering and sedimentation are governed by small-scale object motion in fluid environments. Interfaces play a vital role in the systems' dynamics, because they determine the object-object, object-wall and object-fluid interaction. The term object is used for better distinction with purely numerical particles.

Multi-particle collision dynamics (MPC) is a powerful tool for the simulation of continuum mechanics with internal thermal fluctuations, e.g., see [3, 97]. The particle-based method can be put between the classic scopes of molecular dynamics and continuum mechanics by adding random fluctuations to the continuum field that are still larger than the atomistic length-scale. Despite the different implementations available, a possible workflow consists of three consecutive main steps: streaming, collision and grid shift, see Fig. 2.3. Initially, particles are iniated with mass and starting velocities and the system domain is overlaid with a global collision cell grid. In the first and streaming step, the particles simply propagate with their respective velocity. In the second and collision step, collision of the particles is stochastically mimicked. A variant with stochastic rotation dynamics rotates all particle positions in each cell around a random axis. This computation requires only two random variables for the orientation and a matrix-vector multiplication, per cell. Conservation of energy and momentum are given. Conservation of angular momentum is violated locally, but can be achieved in average or by other means such as repositioning. The proof of an H-Theorem exists to guarantee conver-

gence to the Navier-Stokes equations. Another variant, the Anderson thermostat, picks the random velocities from a Gaussian distribution and can enforce angular momentum conservation by adjusting the velocities to the center of mass and the moment of inertia tensor. The third step performs a grid shift for the conservation of Galilei invariance. Numerical settings such as grid spacing, particle numbers and time stepping will control the effective material parameters. Stochastic properties of the particle positions and velocities determine the mechanical field variables such as temperature and pressure.

Mechanical interfaces play a special role for such numerical tools because they govern the interplay between objects, numerical particles and boundary walls. They determine slip conditions and heat transition, for example. Ghost particles are a possible realization of boundary conditions, which are considered for the collision step by their own mean velocity and temperature-related variance. Suspended objects can also be realized with ghost particles, while other approaches include a decomposition into smaller subparticles or the creation of a rigid bounding mesh. Moreover, their interaction can be evaluated less often for computational efficiency if the particle-particle interaction inside the environmental bulk is governed by a smaller time scale. The cell-based evaluation, the efficient computation algorithms and the rare interaction steps allow for an extreme parallelization of MPC.

The following example of monodisperse PMMA beads of a 60 µm diameter in a water-filled Taylor-Couette cell is simulated with the MP^{2}C framework [232] and compared to experiments with a focus on the contact area between suspended beads and the outer wall. Resulting characteristics such as accumulation density of particles and resting times are relevant for the prediction of transport processes, for instance, at the sea floor or during pumping operations. The simulation settings are tuned to efficiently cover the special situation of classic continuum Navier-Stokes equations with artificial thermal fluctuations.

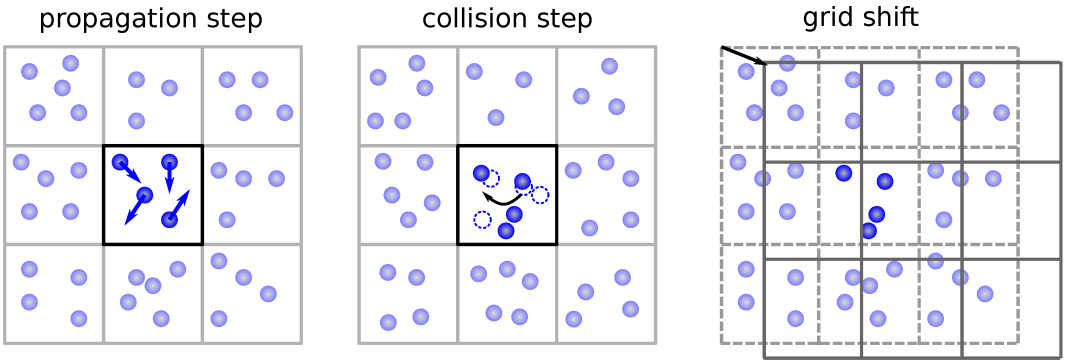

Figure 2.3: Illustration of the multi particle collision algorithm with three typical steps: propagation (with individual particle velocity), mimicking collision (e.g., by random rotation) and grid shift.

Designated publication note

The treatise continues with the following publication(s) as a selected in-depth investigation for the present chapter (it can be found in the concluding chapter of scientific contributions, but may be excluded in public versions for copyright reasons):

K. Schröer, P. Kurzeja, S. Schulz, P. Brockmann, J. Hussong, P. Janas, I. Wlokas, A. Kempf and D. Wolf. Dilute suspensions in annular shear flow under gravity: simulation and experiment. *EPJ Web of Conferences*, 140: 09034, 2017. doi:10.1051/epjconf/201714009034.

3 Sharp interfaces

3.1 Introduction: When zero thickness suffices

Sharp interfaces are probably the most classic approach to describe various observations such as slip planes in crystals, fracture of brittle materials and boundaries in multiphase systems. Their width is often below the mm-scale, which is why they are well approximated by two-dimensional manifolds for many problems on the lab-scale. This chapter will mostly use examples for sharp interfaces that are typically unwanted or demand challenging prediction and control. Sharp surfaces will be studied as a special case of sharp interfaces by neglecting the surrounding material, e.g., free copper surfaces. Also thin coatings may be approximated by a negligible thickness to provide mechanical and other kinds of protection. They can add resistance to different loads such as circumferential stretch, bending or indentation. Mechanical surface treatment can moreover determine the susceptibility to crack initiation in a construction component. Soap bubbles or hollow spheres can even combine two surfaces confining a thin shell into one interface model. The transition appears twice then, for example, doubling the capillarity effect in soap bubbles. Although connected to the enclosed bulk, some surfaces may even behave independently, which is demonstrated in subsequent Sec. 3.2 by a discussion between projection and relaxation of surface deformation.

The mechanics of sharp interfaces that separate two bulk phases can be classified by how they facilitate interaction between the bulk phases in terms of traction and displacement. One possible classification distinguishes coherent interfaces and non-coherent interfaces. The displacement field is continuous across coherent interfaces, e.g., in surface elasticity theory [105]. Non-coherent interfaces allow for a displacement jump, e.g., in cohesize zones or elements. They cover multitudinous mechanical processes and systems themselves. By allowing for a displacement jump but no traction jump, the interface does not even need to remain a two-dimensional manifold. For instance, it allows debonding in layered media [179, 254] or the brittle opening of cracks with two geometrically sharp surfaces [14, 15, 67]. Promiment examples are the three basic failure modes in elastic fracture mechanics (opening, sliding and shearing), for which cohesive zones can provide a theoretical approximation of the stress concentration around crack tips and propagation predictions, e.g., for arterial dissection [226]. True zero-thickness models for such simulations can be found, for example, for brittle crack evolution in the extended finite element method (XFEM) [176]. The propagation of sharp interfaces such as cracks through finite elements is then considered by enrichment with discontinuous fields around the crack. This method benefits from the fact that remeshing can

be avoided to adapt to the moving discontinuity. In addition, various combinations and variants of sharp-interface descriptions [106] have been developed [2]. The opening gap is of course not restricted to void cracks but can also contain a pore fluid in groundwater reservoirs [165] or non-elastic residues of glue or 3d-printed filament [118]. Even more so, closure and contact pose further extensive challenges for interfaces with displacement jumps. Sec. 3.3 below will discuss the case of non-constant displacement jumps in the Helmholtz energy by employing the gradient along the interface. Another, yet related, classification in [132] distinguishes four types of sharp elastic interface models for the purpose of later homogenization. So-called perfect interface models do not exhibit a jump of traction or displacement at all. They can cover simplified phase boundaries or rigid bonding, across which displacement and traction remain continuous. So-called elastic interface models then allow for a traction jump. Cohesive interface models are the third class in this order. Fourth, generalized interface models allow both displacement and traction jumps with individual kinematics and stress contributions of the interface.

3.2 Projection vs. relaxation of surface energies: Theoretical and numerical aspects

The atomistic study of free copper surfaces in Chapter 2 showed that interface deformation can be strongly coupled to the underlying bulk within a finite range. The near-surface rearrangement of atoms, nevertheless, also demonstrated that the surface deformation can contain independent parts such as localized contraction. Surface structures that deviate from perfect planes with severe distortions of the original atomistic bulk structure can result, for example, from surface reconstruction in silicium [46] and gold [250] or see the Wullf shapes of free crystals [239]. Further influences that cause interface-specific mechanics are polarity [98], adsorption [187] and anchoring [136]. Also shells of red blood cells are known for bulk-independent motion which is relevant for their tumbling and tank-treading in blood flow [155, 243].

The subsequent study discusses the difference between projection and relaxation of the underlying, deformation-dependent bulk energy for anisotropic surfaces, Fig. 3.1. The projection of the deformation gradient captures classic in-plane stresses, while the relaxation approach can further relax normal-normal and normal-shear coupling. This opens possibilities for surface relaxation processes that cause geometric disturbances, for example, due to impurities, adsorption, anchoring or polarity. As a result, a projection onto the surface is always a relaxation if anisotropy is superficial, but not vice versa.

Figure 3.1: Projection vs. relaxation of the bulk deformation gradient onto its surface.

Designated publication note

The treatise continues with the following publication(s) as a selected in-depth investigation for the present chapter (it can be found in the concluding chapter of scientific contributions, but may be excluded in public versions for copyright reasons):

C. Sievers, J. Mosler and P. Kurzeja. Projection vs. relaxation of adjacent bulk deformation for surface modeling: Theoretical and numerical aspects. *International Journal of Solids and Structures*, 226: 111084, 2021. doi:10.1016/j.ijsolstr.2021.111068.

3.3 On general imperfect interfaces with spatially non-constant displacement jumps

The mechanical behavior of sharp interfaces becomes particularily interesting for displacement jumps with extra interface-specific stiffness. Such situations occur, for example, during incomplete debonding of 3d-printed layers (Fig. 3.2), partial disintegration between glued components, crazing of polymers or void nucleation along a damage-prone welding seam. Residual connections then still add stiffness to opening and closing motions [184, 189]. The resulting displacement jumps are usually not constant along the open interface, because of spatially heterogeneous loading conditions or degradation of the interfacial connection. Moreover, the interface opens into two surfaces, + and -, which can have different strain states themselves.

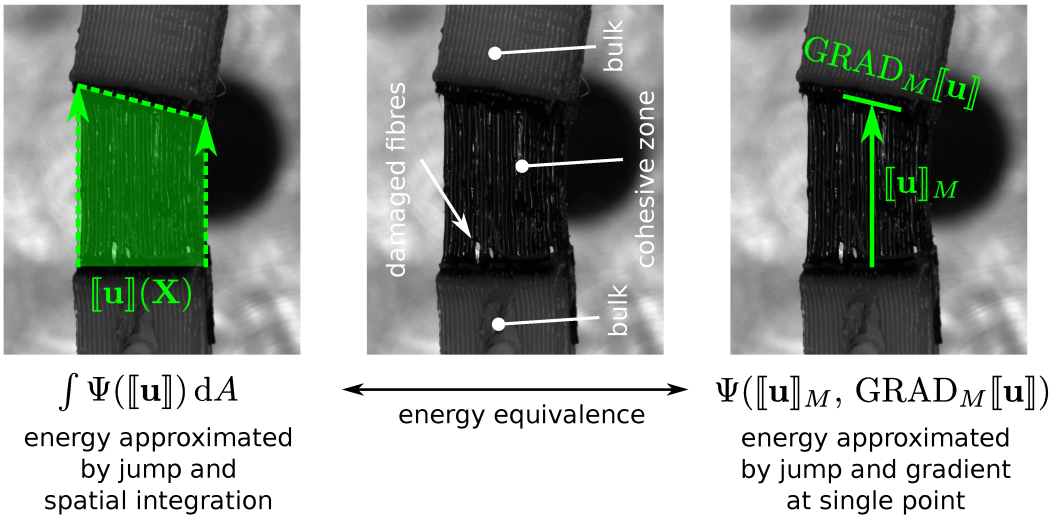

Figure 3.2: Approximation of an affine interface with displacement jump by spatial integration (left) and by a jump with gradient at a fixed point (right). The fully 3d-printed specimen contains a highly flexible, partially damaged thermoplastic elastomere (represented by a cohesive zone) connecting two blocks of polyactide (represented by the surrounding bulk phase at top and bottom) under tilted loading.

In view of the complex situation inside and around the interface, models such as general imperfect interfaces can depend on various parameters, e.g., the displacment jump and deformation gradients on both sides of the opening or in an averaged sense. Like other models, their applicability is a compromise between accuracy and practicability for the problem at hand.

The following investigation compares two approaches to homogenize a spatially affine displacement jump, which is motivated by parametrization by means of a linear finite element. The first approach is a spatial integration of the local displacement jump. The second approach uses the displacement jump and its gradient in one point M, cf. Fig. 3.2. The latter, gradient-based generalized model allows the capturing of additional effects that become relevant for elastic energies of higher than quadratic order. This is highlighted for a 3d-printed specimen with a soft interface.

Designated publication note

The treatise continues with the following publication(s) as a selected in-depth investigation for the present chapter (it can be found in the concluding chapter of scientific contributions, but may be excluded in public versions for copyright reasons):

T. Heitbreder, P. Kurzeja and J. Mosler. On general imperfect interfaces with spatially non-constant displacement jumps. *International Journal of Solids and Structures*, 232: 111068, 2021. doi:10.1016/j.ijsolstr.2021.111068.

4 Diffuse interfaces

4.1 Introduction: Interfaces spreading out physically and numerically

While the previous chapter treated interfaces as sharp two-dimensional objects, the present chapter uses and discusses an alternative approach by means of diffuse interfaces. The view also turns more towards the numerical control of the modeling approaches. Some physical criteria for either sharp or diffuse interfaces have already been discussed in the first two chapters. A physical key condition is the ratio of the real interface width with respect to the other characteristic lengths of the system. The critical question is, for instance, whether the distribution width of micro cracks interferes with the stress fields around a crack tip or whether the rearrangement of molecules at sintering contacts has an impact on the diffusion process through the macroscopic particles. If an interference with the properties of interest cannot be neglected, a diffuse interface description can provide for respective consideration. It specifically allows the accounting for the finite width of cracks, phase boundaries, shear zones, faults, etc.

The first peculiarity of diffuse interfaces is the superposition of adjacent bulk phases. This feature is in contrast to sharp interfaces that fully separate the individual bulk phases from one another. For diffuse interfaces, an order parameter p is often employed to describe the transition from one bulk phase (e.g., $p = 1$) into the other (e.g., $p = 0$). It can be a general distinction and is not restricted to volume or mass fractions, for example. Phase field descriptions rely on this concept and can be applied to many mechanical problems with interfaces. The superposition of bulk phases in diffuse interfaces, however, also requires the distribution of mechanical properties such as energy, deformation, stresses, etc. This can be approached, for instance, by starting from the question of homogenization, or, how to treat a jump of the deformation gradient between both bulk phases, $[\![\boldsymbol{F}]\!]$. Different assumptions applied to this deformation jump yield different homogenization results. A possible classification reads [16, 175]

$$[\![\boldsymbol{F}]\!] \in \begin{cases} \mathbb{R}^{3\times3} & \text{Reuss-Sachs} \\ \{\boldsymbol{a}\otimes\boldsymbol{N}|\boldsymbol{a}\in\mathbb{R}^3,\, \boldsymbol{N}\in S^2\} & \text{rank-one-type relaxation} \\ \{\boldsymbol{a}\otimes\boldsymbol{N}|\boldsymbol{a}\in\mathbb{R}^3,\, \boldsymbol{N}=\nabla p/\|\nabla p\|\} & \text{partial rank-one-type relaxation} \\ \{\boldsymbol{0}\} & \text{Taylor-Voigt.} \end{cases}$$

For example, the Reuss-Sachs assumption allows for static equilibrium with identical stresses in both phases and the Taylor-Voigt assumption fulfills kinematic compatibility by setting the jump to $\mathbf{0}$. The respective constraints associated with Reuss-Sachs and Taylor-Voigt homogenization, however, typically yield lower and upper energy bounds, whereas rank-one and partial rank-one relaxation follow from local and global energy relaxation, respectively.

The role of diffuse interfaces is not restricted to the mere superposition of bulk phases. They are also able to bear interface-specific properties themselves. From an energetic perspective, a prototype interface energy integrated over the total system can read

$$\int_{\mathcal{B}_0} \psi_\Gamma \, f^\varepsilon(p, \nabla p) \, \mathrm{d}V \quad \text{with} \quad f^\varepsilon(p, \nabla p) = \left[\frac{3}{2} \, \varepsilon \, |\nabla p|^2 + 6 \, \frac{1}{\varepsilon} \, p^2 \, (1-p)^2 \right]$$

The factor f^ε can be interpreted as an approximation of the sharp interface's position in the sense of a Dirac-Delta distribution. It depends on the order parameter, p, on its gradient with respect to the reference configuration, ∇p, and on a parameter controlling the width of the diffuse interface approximation, ε. Under suitable conditions, $\inf_\varepsilon \min_p \int f^\varepsilon(p, \nabla p) \, \mathrm{d}V$ converges to the sharp-interface limit of the interface integral in the sense of Γ-convergence [37, 171, 172]. The area-specific Helmholtz energy of the interface ψ_Γ can then be adapted for modeling purposes. Mobility of the phase transformation can be further controlled by a dissipation potential depending on the rate of the order parameter, $\dot{p}$. The temporal evolution of the field variables is then typically classified into conserved and non-conserved types [26]. Conserved field variables such as immiscible phases are governed by the Cahn-Hilliard equations [43]. Non-conserved field variables such as in melts are governed by the Allen-Cahn or time-dependent Ginzburg-Landau equation [6, 7]. The application of phase-field formulations will be demonstrated in the subsequent examples for damage evolution and moreover by topology optimization in Chapter 5.

There are at least two reasons for choosing diffuse interfaces, namely physical and methodological ones. The physical problem can require a diffuse description if there is no sharp distinction between the bulk phases, for example, due to partial diffusion of one phase into the other or due to thermal fluctuations. They can be accordingly covered, for example, by particle-based simulations where distinctions between bulk phases are formed by non-sharp, finite transition zones. Again, such particle-based methods can originate from a physical motivation such as atomistic simulations [55, 251], but they do not need to. Multi-particle collision dynamics [3, 97] and smoothed particle hydrodynamics [173] employ rather artificial particles or kernels that result in interfaces in a stochastically smeared manner by default.

From the other, i.e. methodological, point of view, diffuse interfaces become relevant to overcome problems such as numerical mesh dependence when trying to capture softening effects [194, 224]. For example, damage-induced softening in classic finite-element frameworks yields unphysical localization, i.e., the damaged region depends on the el-

ement size and not on physical parameters. The width of the diffuse interfaces allows the control of the damage zone by acting as a localization delimiter. It can regularize the problem and render it well-posed. Mesh-based continuum simulations are used for diffuse interface descriptions in the context of phase-field [168, 206], micromorphic [90] and level-set methods [51, 186]. Furthermore, there are variants and mixed formulations [211] or integral-based peridynamics [161].

The remaining chapter will analyse regularization in time and space to illustrate advantages and challenges that may arise from diffuse interface descriptions. Sec. 4.2 compares different regularization concepts and how they achieve well-posedness before Sec. 4.3 examines curvature-based interference between numerical regularization and the physical behavior.

4.2 How regularization concepts interfere with (quasi-) brittle damage: a comparison based on a unified variational framework

The softening of materials is known to cause problems for material modeling [18, 194, 224], e.g., the degradation of damaging materials. Interfaces play a vital role because the softening effect yields localization, for instance, in the form of cracks or shear bands. Different types of challenges arise for such phenomena and lead to an ill-posed problem. Firstly, the place of localization is not uniquely determined in initially homogeneous problems. Standard dog-bone test specimens provide a beneficial geometry for elastic investigations, for instance, but make the observation and evaluation of localized degradation difficult in experiments and simulations. Secondly, softening induces instability that can require appropriate regulation, e.g., by experimental feedback control and numerical arc-length schemes. Thirdly, the physical effects take place across a characteristic width that is not considered in standard local models. Instead, localization in mesh-based simulations of local models appears by softening of single elements and is thus dictated by the numerical element size, but not by the physical length scale, cf. Fig. 4.1.

Diffuse interfaces are one possibility to introduce the missing length scale. The ill-posed problem becomes regularized. The term regularization can have a different meaning or focus, though, depending on the research area. Mathematical studies often approach regularization in the sense of singularities, missing differentiability or a lack of uniqueness and can also involve convergence of penalty formulations or solution sequences. By way of contrast, engineering studies often focus on implied problems such as numerical instabilities, branching of solutions and mesh dependency. Regularization schemes moreover can be based on real physical behavior, e.g., viscosity. Yet, a regularization scheme can also be motivated as a mere numerical requirement for the control of the length scale. Such artificial regularization, however, should at least account for

scale separation to prevent an interference with the predicted physics (it must be small enough to not affect the mechanical response) and with the mesh resolution (it must be large enough to be resolved).

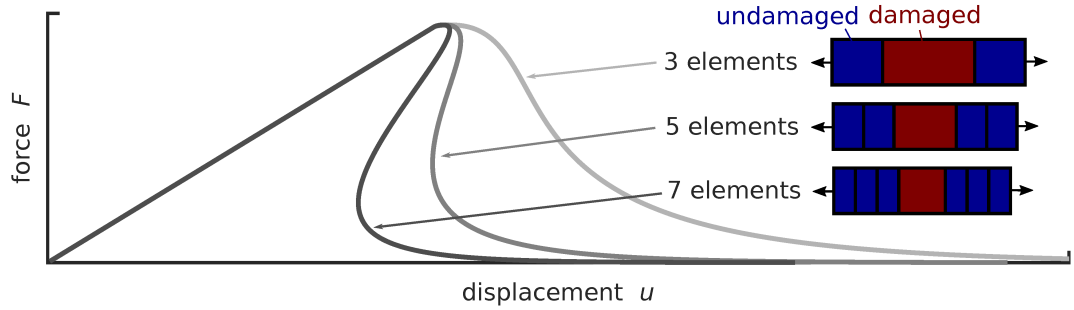

Figure 4.1: Normalized force-displacement curve for illustration of mesh dependence of a local damage model. The test is a one-dimensional bar under uniaxial loading with three, five and seven elements for spatial discretization. The center element has an imperfection in the form of a slight initial degradation. Insets show the damage distribution at the final stage of virtually complete failure.

The following investigation compares three different regularization methods, the fracture energy concept, viscous regularization and spatial gradient-based regularization in a micromorphic framework. The fracture energy concept yields a constant fracture energy but the underlying system of partial differential equations remains ill-posed. The viscous regularization yields a well-posed problem but artificial viscosity can add a bias to unloading and fracture thickness due to locally heterogeneous loading rates. The well-posed micromorphic regularization does not show this interference with the underlying physics by paying the price of higher computational costs.

Designated publication note

The treatise continues with the following publication(s) as a selected in-depth investigation for the present chapter (it can be found in the concluding chapter of scientific contributions, but may be excluded in public versions for copyright reasons):

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4.3 Interference of gradient-regularization with interface curvature

The use of continuous, auxiliary fields allows for a beneficial description of microstructure evolution and interface motion under different driving forces, e.g., mechanical, thermal, electric or magnetic fields. As mentioned before, it also allows for regularization via the diffuse interfaces. The respective frameworks usually employ a gradient extension that connects to the extra length scale. Where and how to put the gradient extension is an ongoing research task [219]. Phase-field implementations [168, 170], for example, can account for damage by a global phase-field variable φ. Regularization is then achieved by a non-local dissipation term, which does not only employ the field variable and its rate, but also its gradient $\nabla\varphi$. The non-local dissipation part or surface energy density rate can take the form, for instance, $g_c/l\,[\varphi\,\dot{\varphi} + l^2\,\nabla\varphi\,\nabla\dot{\varphi}]$. The two components open the possibility for calibration of both fracture energy and regularization length. Micromorphic implementations [84], as another example, allow the coupling between an internal damage variable α and a global auxiliary field φ by means of a penalizing micromorphic energy. One possibility to obtain spatial regularization is then by adding a gradient term of the auxiliary field to the energy for spatial regularization. The penalty and the gradient term can take a form such as $c\,[\alpha - \varphi]^2 + c\,l^2\,\|\nabla\varphi\|^2$. In both cases, the governing term due to the gradient extension in the balance equations takes the form $\nabla \cdot \nabla\varphi$. Gradient-based regularization shows individual benefits, e.g., being rate-independent and not interfering with the time scales of the physical processes. Initially aiming for a control of the diffuse interface width, however, it also affects the interface evolution by a curvature-related term.

The subsequent investigation examines the methodological side effect of gradient enhancement on curved damage fields. Its origin can be highlighted by using a split of the gradient term into its length and its normal direction as $\nabla\varphi = \|\nabla\varphi\|\,\boldsymbol{n}_\varphi$. The relevant gradient-induced term inside the balance equations then transforms into

$$\nabla \cdot \nabla\varphi = (\nabla\|\nabla\varphi\|) \cdot \boldsymbol{n}_\varphi + \|\nabla\varphi\| \underbrace{\nabla \cdot \boldsymbol{n}_\varphi}_{=:\,-2\,\kappa}\,.$$

The first part controls the width of the diffuse interface's transition zone in normal direction. The second term is linked to the interface's curvature κ. This second influence may not be intended, though, and can lack a physical origin. Curvature-dependent effects are known but often restricted to very small scales. The following study hence discusses possible implications with respect to quasi-brittle damage evolution.

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The treatise continues with the following publication(s) as a selected in-depth investigation for the present chapter (it can be found in the concluding chapter of scientific

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5 Utilizing interfaces for the design of structures

5.1 Introduction: Turning defects into opportunities

The interfaces discussed in the previous chapters were mostly inspired by naturally predetermined or even undesired processes. Among more practical examples, new surfaces automatically appear as a result of abrasive treatment [217] and the path of cohesive zones in hip replacements is guided by the intact biological structure [246]. Cracks, as a prominent example of undesired interfaces, typically reduce the lifetime of components [91], contact interfaces are prone to wear [128] and earthquake-induced liquefied layers of soil can result in hazardous damage [76].

Interfaces, nevertheless, also open various opportunities and the present chapter intentionally turns the view towards their beneficial sides. Grain boundaries, for instance, can pin dislocations and increase the yield strength of a material by hindering plastic deformation. The Hall-Petch relation accordingly predicts an increase in yield stress for smaller grain sizes and larger interfacial area, up to a material-specific limit [110, 196]. Control of fluid flow is also made possible by the role of interfaces as boundaries on larger geophysical environments [164], for the migration and distribution of highly toxic nonaqueous phase liquids [165] or inside microfluidic devices for mechanical modeling of a tumor environment and real-time screening of drug efficacy [42]. Interfaces can also help to filter or mitigate sound signals. Air curtains, for instance, are one approach to reduce broadband sound pulses that are generated by hammer blows of underwater pile drivers. The surface tension of air-water interfaces helps to stabilize the air bubbles for sound reflection and absorption. The surface design of acoustic foam also reduces sound amplitudes, e.g., attenuating air-borne waves inside buildings [79]. In phononic crystals, gyroscopic effects can moreover allow one-way elastic surface-bound edge waves [248]. The skin of animals is also a remarkable surface or interface, when considered to be in contact with another object. Its elasticity under severe tension and creasing allows for an extremely large range of motion of the underlying joints. Also the regeneration of biological tissue is just another of the many noteworthy capabilities. For example, cells can use alterations of the mechanical condition effectively as self-adjusting means of communication [24].

Apart from their mechanical role, interfaces also see numerous beneficial applications in other fields such as thermal insulation [145], fluid regulation [127], eletromagnetic

wave absorbers [188] or optical properties in solar cells [47]. The design of mechanical and other properties is typically strongly coupled, which leads to a multi-physics problem in many applications.

The following studies highlight particular aspects that can be achieved via interface-based design, namely, beneficial instabilities and topology optimization. The severe morphological deformation of instable structures studied in Sec. 5.2, for instance, allows for folding or tuning of phononic band gaps in highly elastic, porous strutures [221] and honeycomb structures for energy absorption in crashworthy helicopter seats [64]. Topology optimization in Sec. 5.3 constitutes a field that vividly demonstrates the interplay between bulk materials and interfaces. The evolution of size and shape is indeed not only governed by the bulk parameters but also by those of the interfaces [77]. Grain growth, for example, is determined by minimizing internal energy via reduction of the grain boundary area, yielding control of strengh, toughness, creep resistance and extraordinary properties such as exceptionally large ductilities [126]. Natural examples of interface-driven topology optimization is the cell formation and stability of foam [92] and epiphyseal growth plates that affect longitudinal growth of long bones following cartilage forming, calcification, degradation and replacement by osseous tissue [198, 201].

5.2 Harnessing instable structures for dissipative fluid flow

More than half a century ago, Biot's seminal work on elastic waves in fluid-saturated porous solids [27, 28] allowed a reliable prediction of wave speeds for saturated poroelastic media. Interfaces play a vital role for the exchange of momentum in these systems such as rocks or bones. The attenuation however seemed to be underestimated. The main dissipative process was assumed to be due to inertia-driven decoupling of the viscous fluid. Another explanation was later found in the form of so-called squirt flow or local flow [69, 103, 183, 200]. It matches experimental observations in complex systems better in terms of much higher attenuation at lower frequencies. Moreover, it is known to be severely affected by the geometry of interfaces of fractures or cavities, respectively [38, 49]. Indeed, it relies on the heterogeneous compliance of pore space. Fluid is displaced locally from softer to stiffer pores. One possible situation is the intersection of perpedicular fractures. One fracture may be closed upon directional compression and squirts fluid into the other. This associated time scale depends on the ratio of viscous forces to elastic forces and yields lower frequencies than classic Biot-type flow.

While the effect of local flow has been discovered in geological materials [4, 5], its characteristics — high attenuation at low frequencies — are promising for artificial environments, e.g., buildings prone to earthquakes or propellant tanks with low resonsance frequencies. Geological materials yet share a constraint that can be found for many low-frequency dampers, that is large mass and size. Interestingly, novel material classes emerge as a light-weight alternative in the form of architected elastomeric structures. So-

called metamaterials, for instance, can be designed to achieve a negative Poisson's ratio or tunable acoustic band gaps [11]. While instabilities usually carry negative connotations, they can hence be used beneficially thanks to their severe changes in morphology, e.g., see Fig. 5.1. Moreover, they can provide a light weight and extremely heterogeneous interface deformation compared to geological materials.

The following two studies hence aim at combining the two previously mentioned structural effects. They harness the local-flow effect from geological materials in artificially designed structures. This allows attenuation at very low frequencies of a few Hz without the restriction of large masses or sizes of conventional dampers. The relevant attenuation frequencies are instead determined by a competition between viscous and elastic contributions that can be controlled by design and the buckling state.

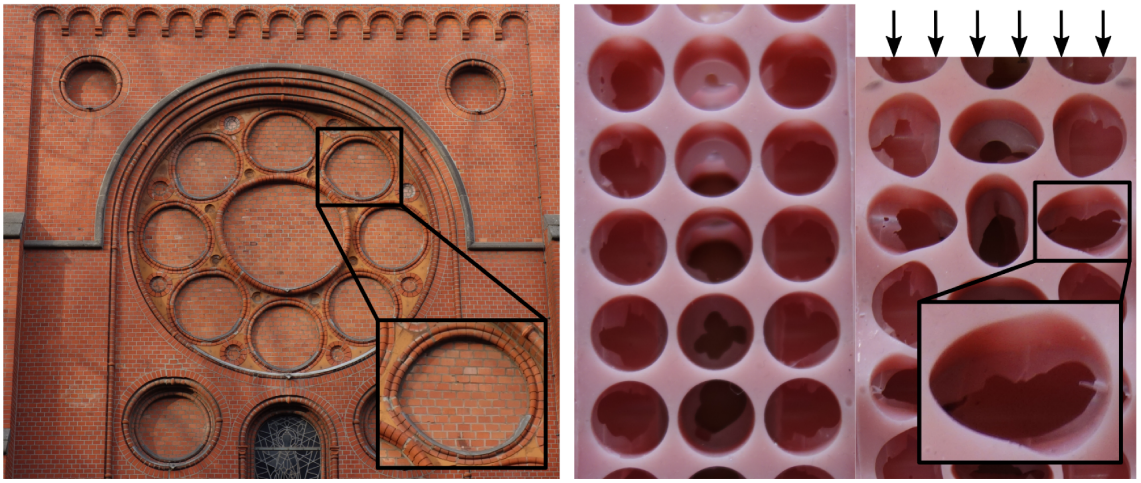

Figure 5.1: Buckling instablities in architected structures: undesired in the ornaments of the St. Joseph Church in the city center of Bochum, Germany (left) and desired in metamaterials cast from duplication silicone (right, undeformed/deformed).

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T. Cohen, P. Kurzeja and K. Bertoldi. Architected squirt-flow materials for energy dissipation. *Journal of the Mechanics and Physics of Solids*, 109: 22-33, 2016. doi:10.1016/j.jmps.2017.08.003.

P. Kurzeja and B. Quintal. Harnessing local flow in buckling pores for low-frequency attenuation. *International Journal of Solids and Structures*, 285: 112508, 2023. doi:10.1016/j.ijsolstr.2023.112508.

5.3 Cahn–Hilliard phase-field theory coupled to mechanics: Fundamentals, numerical implementation and application to topology optimization

Topology optimization is a rich field in terms of application and methodology [21] and covers, amongst others, density-based solid isotropic material with penalization (SIMP), hard-kill bidirectional evolutionary structural optimization (BESO) or level-set methods [59, 223]. The interaction between bulk phases and interfaces often determines the resulting structure, see Fig. 5.2. The phase-field method has emerged as a convenient numerical tool for the smooth description of such problems. Applications are found for spinodal decomposition, fracture mechanics and so-called TRIP and TWIP steels with transformation-induced and twinning-induced plasticity. It moreover allows the fulfilling of physical constraints such as a sharp-interface limit in the sense of Γ-convergence and conservation of mass. Also refer to the homogenization discussions of diffuse interfaces in Chapter 4.

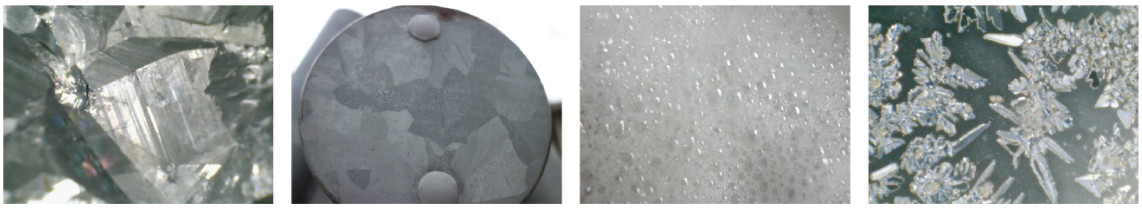

Figure 5.2: Structures evolved with distinct boundaries from left to right: quartz, a metallic ridgepole, soap bubbles and frost crystals.

The parameter p in many phase-field descriptions of Allen-Cahn type evolves such that the stored energy is minimized [6, 7]. The variational framework below will show that its rate $\dot{p}$ indeed correlates with a descending energy (variation) of bulk phases and interfaces (with respect to p) until the driving force vanishes. In other words, material is removed from regions bearing heavy loads. Allen-Cahn formulations are however not conservative, while many relevant applications aim at opimization for a predetermined amount of material for the sake of weight or cost limitation [21]. This can be enforced by a diffusion equation, to mention one well-known approach, which leads to a Cahn-Hilliard type formulation [43]. It relates the rate $\dot{p}$ to the Laplacian of the energy variation of bulk phases and interfaces with respect to p.

The subsequent investigation provides a variational framework to couple the Cahn-Hilliard phase-field theory to continuum mechanics. It specifically illustrates how topology optimization emerges automatically from the variational formulation. The standard Cahn-Hilliard phase-field model tries to minimize the free energy of the system and

shifts material from loaded to unloaded regions. For the sake of topology optimization, the signs of two terms must be changed, namely those related to bulk energy and to external loads. It can be understood as a different orientation of the driving force. The interface evolution remains unaffected and provides regularization of the problem. The proposed reformulation will be physically explained by the use of Clapeyron's theorem for alternative definitions of compliance in linear-elastic systems.

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A. Bartels, P. Kurzeja and J. Mosler. Cahn-Hilliard phase field theory coupled to mechanics: Fundamentals, numerical implementation and application to topology optimization. *Computer Methods in Applied Mechanics and Engineering*, 383: 113918, 2021. doi:10.1016/j.cma.2021.113918.

6 Interfaces for information transfer across scales

6.1 Introduction: What interfaces can tell us

While Chapter 2 opened the scientific investigations by predicting the behavior of a single interface, this chapter shall close the treatise by predicting the behavior of interface ensembles. It does so by aiming at the particular question of what interfaces can tell us about a mechanical system?

From a mere geometrical perspective, interfaces are a canonical extension of volume fractions, which are probably the most basic information on a multiphase system's composition. Volume fractions can be derived, for instance, from grain-size distribution curves of sediment [54], point counts and other measurements in stereology [122] or nano X-ray fluorescence imaging of zinc distribution in cucumber plants [244]. Interfaces then add a next level of geometric information that can be relevant to contact, friction, crack initiation or diffusion. For example, the adhesion of powder with rough particle surfaces [197], the energy dissipation capacity of bone between fibril arrays [216], the electrochemical behavior of rusted steel [156] and sintering [138] depend on the size and shape of the interfaces involved. Very often, however, detailed information regarding the interface evolution in space and time is not available. Using or even gathering this information can be demanding or impossible for systems with multiple interfaces, let alone the interference between measurement and the physical system. Dealing with scarse information is sometimes unevitable due to experimental, numerical or analytical constraints. Ensembles of interfaces thus often require a simplification, e.g., in the form of a homogenized description. The previous views on homogenization towards interfaces (e.g., atomistic descriptions and excess properties in Chapter 2) or homogenization at interfaces (e.g., phase averages in Sec. 5.3) are however too detailed for the present chapter's focus on interface ensembles.

Multiple interfaces are found in many studies of scale effects and designed interfaces. A very prominent role in this regard is found for the interpretation of damage in terms of pores or voids. The size and shape of the pore boundaries can affect anisotropic degradation, e.g., for damage or plastic evolution in steel [104, 151, 203]. The interface can also be used to systematically tune effective parameters by design. Design studies are found for systematic periodic homogenization, e.g., in stiffness parameters for structures with inclusions [132] or the Bloch analysis of instability-induced pattern transformations [131], the principle of virtual work as a rational framework for pantographic design [61]

as well as for stochastic homogenization [180], e.g., moving interfaces with oscillatory velocity [48] or viscoplastic polycrystals [148]. Interfaces within an RVE are hence a valuable option in microstructural design when combined with computational homogenization [50, 83, 88].

A systematic key variable for the quantification of interface ensembles is the interface to volume ratio, or interfacial areas, e.g., a_{wn} between a wetting (w) and a non-wetting (n) phase. They can be derived by spatial averaging from the interface area per reference volume. Such averaged values provide accessibility by a reduction of accuracy but neglect several microscopic features. The curvature field of the interface is not preserved, for instance. However, building upon interfacial areas as a variable can still be profitable. Within the class of mixture theory for superposed continuum phases and the theory of porous media [20, 36, 52, 56, 71], the threepart work of Hassanizadeh & Gray [113–115] provides a thermodynamically rigorous two-scale framework that depicts the use of interfacial areas very vividly. The following example of capillarity shall thus be adressed for an introducing illustration of how a_{wn} can be used as useful macroscopcic information.

Starting from the microscale, the Young-Laplace equation relates capillary pressure p^c proportionally to surface tension γ_{wn} and curvature κ. Curvature, nevertheless, is not conserved during homogenization to the macroscale. A multiscale framework allows the introduction of macroscopic capillary pressure from a thermodynamic perspective instead. Focusing on oftentimes applicable assumptions such as isothermal conditions and negligible solid deformation then yields an illustrative approximation of the macroscopic capillary pressure. At equilibrium, it can then be defined as the pressure difference between wetting fluid (w) and non-wetting fluid (n), $p^{\mathrm{w}} - p^{\mathrm{n}}$. Moreover, it can be related to the derivative of the interfacial free energy with respect to the volume fraction of the wetting fluids, $\partial\Psi_{\mathrm{wn}}/\partial n_{\mathrm{w}}$, by using the entropy inequality [116, 117] (similar to the energentically dual pair of pressure and volume changes in bulk phases). Assuming the interfacial free energy to be the product of constant surface tension and variable interfacial areas in agreement with microscopic observations, $\Psi_{\mathrm{wn}} = \gamma_{\mathrm{wn}}\, a_{\mathrm{wn}}$, then yields

$$p^c \approx \frac{\partial \Psi_{\mathrm{wn}}}{\partial n_{\mathrm{w}}} = \gamma_{\mathrm{wn}} \frac{\partial a_{\mathrm{wn}}}{\partial n_{\mathrm{w}}}.$$

The resulting equation is in agreement with macroscopic scenarios in hydrogeology, e.g., when a pressure difference is required for drainage or imbibition of groundwater. Even more so, the last term $\partial a_{\mathrm{wn}}/\partial n_{\mathrm{w}}$ is the macroscopic counterpart of curvature as it describes the change of surface area with respect to volume fraction. The evolution of interfacial areas can hence contain significant information that may not be expected from their simple definition. Interfacial areas have since then been successfully implemented in further extensions, e.g., as a missing variable to account for hysteresis effects of drainage-imbibition curves [134, 181].

The following investigations will first discuss how interface-dominated physics can be used to relate microscopic gas bubble oscillations efficiently to acoustic signals for

destruction-free characterization in Sec. 6.2. The investigation in Sec. 6.3 then raises the question as to how interfacial areas can be sufficient information to transfer to the macroscale. This is answered by adopting the method of Rao-Blackwellization from mathematical statistics. The resulting framework is finally used to improve predictions in imperfect artificial neural networks.

6.2 Interface dynamics for ultrasound characterization

Ultrasound characterization stands out as a desctruction-free method with flexibility under laboratory and operational conditions. Ultrasound signals interfere with interfaces in many ways and so accordingly gave rise to various techniques for detection and aquisition of information. The application spectrum strongly depends on the ratio of acoustic wave length to the interface's length scale. Reflection at larger cracks, for instance, allows the detection of damaged zones [66]. More complex systems affecting our environment and ourselves can also successfully be studied with ultrasound techniques. Sonograms, for example, allow an insight into the evolution of an embryo [236]. Allowing much lower frequencies for a moment, earthquake reflections create a picture of the earth's inner composition [119]. Mechanical interfaces guide the waves by affecting reflection and transmission. Acoustic resonance can moreover be used to relate to threaded interfaces [212]. At higher frequencies, the interference between finer stuctures and ultrasound signals often no longer leads to single, clear measurements. Instead, the attenuation or dispersion of signals can relate to the structure's characteristic size, e.g., in the form of absorption or scattered diffusion of the signals [107]. A coupling to electromagnetic waves is also available [30, 205, 218].

The following investigation aims at the characterization of a bubbly liquid inside an elastic matrix via ultrasound. Such systems range from batteries to rocks and drying plants [130, 164, 231]. The subsequent numerical study specifically aims at air-bubbles in liquid-saturated rock. They do not only involve three types of bulk phases but also interfaces with completely different roles. The solid-liquid interfaces determine the viscous coupling, while the liquid-gas interfaces induce capillary effects. In contrast to most of the previous quasi-static investigations, the interface dynamics will also take a prominent role.

A special homogenization approach is used by treating the enclosed gas bubbles as individual oscillators that exchange momentum via their interfaces. They are not accounted for as a single, averaged modification of the elastic, viscous or density tensor. Instead, the bubbles' distribution of eigenfrequencies and damping factors can be considered individually or in a statistically smeared manner. This preserves relevant information for the acoustic response. It allows the relating of the signals to the inner structure and depends heavily on the interface mechanics. Attenuation of the wave signals and resonance frequencies relate to the Womersley number (ratio of transient inertial forces to viscous forces for pulsating flow) and the capillary number (ratio of viscous forces

to capillary forces). This interface-dominated influence is considered by the mass, the damping and the stiffness of each bubble.

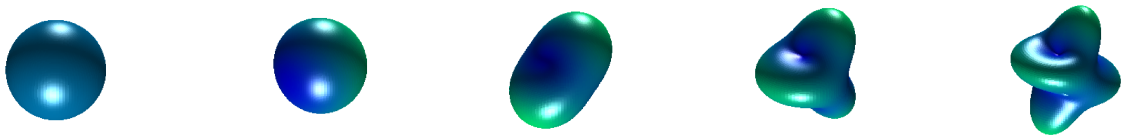

Figure 6.1: Oscillations modes of a compressible gas bubble with surface tension in a surrounding liquid. The first mode is expansion while the second is translation.

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The treatise continues with the following publication(s) as a selected in-depth investigation for the present chapter (it can be found in the concluding chapter of scientific contributions, but may be excluded in public versions for copyright reasons):

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6.3 Sufficient information transfer of interfaces

Information transfer across scales is not only present in mechanical multiscale modeling, but also in statistical modeling [60]. Both indeed share some striking similarities as illustrated by the list of the involved steps in Tab. 6.1. The last two entries mark a statistical concept for the improvement of predictions, including the step of Rao-Blackwellization. It is not explicitly familiar in mechanical modeling, though. The Rao-Blackwell theorem uses sufficient information to improve the prediction of a model parameter, e.g., the mean or the standard deviation [31, 124, 207, 220]. It starts with an initial (and possibly even crude) estimator θ_0 from the sample values X. Knowing what information $\mathcal{S}$ is sufficient to use from the sample, the conditional expectation $\mathbb{E}(\theta_0(X)|\mathcal{S}(X))$ is typically a better estimator and never worse. The algorithm ensures that the new estimator will provide the same prediction from the same sufficient information value $\mathcal{S}$, independent of underlying variations in the data of X.

The similarities of mechanical multiscale modeling and statistical modeling allow the adoption of the Rao-Blackwell theorem to mechanical modeling. This is not only due to the conceptual structure but also due to the mathematical formalism. Averaging and expected values can both be interpreted as weighted integrals over underlying states. As one result, they allow the definition of an associated error norm and an algorithm for the improved prediction. The definition of sufficiency must yet be renewed for me-

Table 6.1: Comparison of exemplary steps in multiscale mechanical modeling and statistical modeling.

step	mechanical multiscale modeling	statistical modeling
origin	microscopic process	randomized process
model	macroscopic model	statistical model
unknowns	macroscopic model parameters	statistical model parameters
determined by	physical relationships	estimators
from	predetermined parameters	random samples
via	homogenization	expectation
improved by	$\hookrightarrow$	Rao-Blackwellization
via		sufficient information

chanical problems. Statistical sufficiency can be related to a characterization by the Fisher-Neyman factorization theorem, for instance. Sufficiency in mechanical modeling, in contrast, must derive from physics-based constraints. These can include symmetry conditions, dimensionless classification or the coefficients in a set of partial differential equations. Knowledge about the solution is not necessary. It is only important to know what sufficient information uniquely fixes the solution. The idea of sufficient information reverses the search for more comprehensive models towards the necessary components. It hence serves similar purposes as the areas of model order reduction and surrogate modeling [17, 208]. Among them, it yet stands out as a tool that can improve even crude initial estimators and deals with small amounts of information.

The next investigations thus present how Rao-Blackwellization can be adopted to mechanical problems and how it can be combined with artificial neural networks, which heavily depend on the data basis available. Interfaces will be a central part during these investigations, because adding interface information can be sufficient in order to describe several new effects. Employing sufficient interface information in homogenized capillary systems, for instance, proves to be beneficial for the description of drainage-imbibition curves. Using sufficient information in neural networks, for example in terms of stresses or strains, moreover helps to reduce noise and overfitting. Even more so, it can improve crude initial estimations of sparse data.

Designated publication note

The treatise continues with the following publication(s) as a selected in-depth investigation for the present chapter (it can be found in the concluding chapter of scientific contributions, but may be excluded in public versions for copyright reasons):

P. Kurzeja. The criterion of subscale sufficiency and its application to the relationship between capillary pressure, saturation and interfacial areas. *Philosophical Transactions of the Royal Society A*, 472: 20150869, 2016. doi:10.1098/rspa.2015.0869.

G.-L. Geuken, J. Mosler and P. Kurzeja. Incorporating sufficient physical information into artificial neural networks: a guaranteed improvement via physics-based Rao-Blackwellization. *Computer Methods in Applied Mechanics and Engineering*, 423: 116848, 2024. doi:10.1016/j.cma.2024.116848.

7 Conclusion

Interfaces are ubiquitous. A great number of natural and artificial systems would not achieve their mechanical functionality without them. They are indispensable for slip in crystals, conductivity in reservoir rock, fracture in glass, gas exchange in alveoli, cohesive bandages, stability of foam and much more. Their roles are as multifaceted as their appearence. We shall recapitulate them from the three viewpoints as motivated in the very beginning.

Modeling of interfaces with molecular simulations showed that the definition of an interface is not straight-forward. Properties such as width, mass, stress or energy are not trivially defined. An energetic approach can provide a rigorous homogenization for that purpose from molecular to continuum mechanics. Dynamic particle-based approaches can moreover account for effective thermal exchange across interfaces. Pure continuum interfaces are then frequently found to be approximated either by sharp or by diffuse descriptions. While the diffuse width can have a physical origin, the choice is often also a matter of the modeling framework and numerical implementation. Models for ensembles of interfaces finally reduce their complexity to effective parameters like interfacial areas or tortuosity. Interface models are numerous in such a way that they intersect many disciplines, of which engineering and physics were prominently presented.

Control of interfaces is pursued for natural and artificial interfaces alike. It was shown that the path of freely evolving interfaces must be controlled to mitigate the impact of damage zones. From the methodological perspective, the numerical behavior of interfaces must also be controlled to limit interference with the overall physics, e.g., the curvature-dependence of higher-order gradient theories. Adjusting their energy also controls their evolution and thus the materializing topology of structures. The analysis of buckling patterns demonstrated how interface design controls their deformation modes and induced flow of pore fluid. The effects of their control underlines their role as a mediator between the bulk phases.

Opportunities arise from interfaces as inevitably as do risks. Both sides shall be emphasized here together, because some areas of application approach interface problems only from one direction or the other. Evolving cracks, on the one hand, constitute a prominent ecological and economic risk. Evolving phase boundaries, on the other hand, were shown to guide the evolution of optimized micro structures. Non-uniform distributions of interfaces can moreover trigger squirt flow in fluid-filled structures and thus enable acoustic characterization of ground earth. The opportunity of characterization is also possible due to capillarity-driven resonance in residually saturated media.

Interfacial areas can eventually provide information in static cases as was shown by their role as an additional parameter to resolve hysteresis effects or to enrich the data basis of artificial neural networks.

The in-depth studies already derived research questions for future continuation. From the broader view, it remains to conclude that the challenges particular to interfaces can also guide their potential use in future investigations. Their dominance on small scales may complicate their fabrication and investigation. However, this also makes it possible to exceed the limits of pure bulks. Information and characterization of interfaces can be continued by network analysis, which is not possible for structureless bulks. Fluid-structure interaction may be harnessed further when inspired by other effects in natural systems, either anorganic or organic. Curvature effects of higher order can be promising for topology control when employing Gaussian curvature in the future. Concluding concisely, interfaces are more than simple defects of bulk phases. They can open new avenues by harnessing their modeling, control and opportunites.

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