@article{Steinmann2008,

author = {Paul Steinmann},

title = {On boundary potential energies in deformational and configurational mechanics},

journal = {Journal of the Mechanics and Physics of Solids},

volume = {56},

number = {3},

pages = {772 - 800},

year = {2008},

issn = {0022-5096},

doi = {https://doi.org/10.1016/j.jmps.2007.07.001}

}

This contribution deals with the implications of boundary potential energies, i.e. in short surface, curve and point potentials, on deformational and configurational mechanics.

Inspired by an atomistic/molecular picture of materials, which is of particular relevance in the realm of nanomechanics, it is obvious that the boundary of a continuum body (or an interface between subparts of a continuum body) displays different properties as compared to its bulk. This phenomenon is usually modelled in terms of surface/curve tension.

A first comprehensive, purely mechanical approach towards the treatment of elastic material surfaces was proposed by Gurtin and Murdoch (1975). Here, besides providing all the necessary results for the kinematics and balance laws for surfaces, in particular the tensorial nature of surface tension within deformational mechanics was established.

Contributions almost entirely devoted to the configurational mechanics of interfaces are by (Gurtin (1995,2000), which derive the relevant surface balance equations essentially from non-standard (material) observer invariance.

The philosophy of this contribution is somewhat different from the above references: within a variational (hyperelastic) framework configurational forces are defined as capturing energetic changes that go along with so-called material variations, i.e. configurational changes. Thus the energy release or rather the dissipation resulting from material variations, i.e. variations at fixed spatial placements, is considered.

A main thrust of this contribution is to emphasize the striking duality of (but also the difference between) the (localized) force balances at surfaces/curves/points within deformational and configurational mechanics, whereby especially boundary potentials are taken into account.

@article{Javili2009,

title = "A finite element framework for continua with boundary energies. Part I: The two-dimensional case",

journal = "Computer Methods in Applied Mechanics and Engineering",

volume = "198",

number = "27",

pages = "2198 - 2208",

year = "2009",

issn = "0045-7825",

doi = "https://doi.org/10.1016/j.cma.2009.02.008",

url = "http://www.sciencedirect.com/science/article/pii/S0045782509000802",

author = "A. Javili and P. Steinmann",

keywords = "Boundary potentials, Surface tension",

}

This contribution deals with the implications of boundary potential energies on the two-dimensional deformations of solids in the framework of the finite element method. Common modelling in continuum mechanics takes exclusively the bulk into account, nevertheless, neglecting possible contributions from the boundary. However, boundary effects sometimes play a dominant role in the material behavior, the most prominent example being surface tension.

Moreover, in material processing, the boundary of material is fre- quently exposed to, e.g. oxidation, ageing, grit blasting, plasma jet treatment, etc., thus obviously resulting in distinctively differ- ent properties in comparatively thin boundary layers. Likewise coating materials with thin films result clearly in different proper- ties at the boundary. These effect could phenomenologically be modelled in terms of boundaries equipped with their own potential energy.

@article{SteigmannOgden1999,

title = {Elastic surface-substrate interactions},

journal = {Proceedings of the Royal Society of London A},

volume = {455},

pages = {437 - 474},

year = {1999},

author = {D. J. Steigmann and R. W. Ogden}

}

A theory for three-dimensional finite deformations of elastic solids with conforming elastic films attached to their bounding surfaces is described. The Gurtin–Murdoch theory incorporating elastic resistance of the film to strain is generalized to account for the effects of intrinsic flexural resistance. This modification yields a model that can be used to describe equilibrium deformations in the presence of compressive- surface stress fields.

Gurtin & Murdoch (1975) presented a rigorous theory of the mechanics of surface- stressed solids based on the idea of a two-dimensional membrane bonded to the surface of a bulk substrate material. Their work generalizes the classical notion of surface tension in solids and allows for the systematic theoretical description of general states of residual surface stress.

The Gurtin–Murdoch theory was motivated in part by empirical observations pointing to the presence of compressive surface stress in certain types of crystals.

@article{GurtinMurdoch1978,

title = {Surface stress in solids},

journal = {International Journal of Solids and Structures},

volume = {14},

number = {6},

pages = {431 - 440},

year = {1978},

issn = {0020-7683},

doi = {https://doi.org/10.1016/0020-7683(78)90008-2},

author = {Morton E. Gurtin and Ian A. Murdoch}

}

More generally, microscopic considerations predict the presence of surface stress whenever a new surface is created.

@article{GurtinMurdoch1975,

title = {A continuum theory of elastic material surfaces},

journal = {Archive for Rational Mechanics and Analysis},

volume = {57},

number = {4},

pages = {291 - 323},

year = {1975},

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A mathematical framework is developed to study the mechanical behavior of material surfaces. The tensorial nature of surface stresses established using the force and moment balance laws. Bodies whose boundaries are material surfaces are discussed and the relation between surface and body stress examined.

@article{Hong2008,

title = {A theory of coupled diffusion and large deformation in polymeric gels},

author = {Wei Hong and Xuanhe Zhao and Jinxiong Zhou and Zhigang Suo},

journal = {Journal of the Mechanics and Physics of Solids},

volume = {56},

number = {5},

pages = {1779 - 1793},

year = {2008},

issn = {0022-5096},

doi = {https://doi.org/10.1016/j.jmps.2007.11.010}

}

Polymeric gels are used in diverse technologies, including medical devices (Jagur-Grodzinski, 2006), drug delivery (Duncan, 2003; Fischelghodsian et al., 1988; Jeong et al., 1997; Langer, 1998), tissue engineering (Luo and Shoichet, 2004; Nowak et al., 2002), and stimuli-sensitive actuators (Beebe et al., 2000; Dong et al., 2006; Sidorenko et al., 2007).

Field theories of mass transport in elastic solids date at least back to Gibbs (1878), who formulated a thermodynamic theory of large deformation of an elastic solid that absorbs a fluid, assuming that the solid and the fluid have equilibrated. Biot (1941) combined a similar thermodynamic theory with Darcy’s law to model the motion of a fluid in a porous elastic solid. The resulting theory, known as poroelasticity, has been used to analyze phenomena ranging from compaction of soils to deformation of tissues. Rice and Cleary (1976) presented several fundamental solutions in poroelasticity.

Several groups have formulated theories specifically to couple mass transport and deformation in gels, invoking various conceptual pictures (e.g., Tanaka and Fillmore, 1979; Durning and Morman, 1993; Dolbow et al., 2004, 2005; Tsai et al., 2004; Li et al., 2007). Both the concepts and the materials are sufficiently complex such that ample room exists for additional theoretical work to connect principles of mechanics, thermodynamics, and kinetics to experiments and to molecular models.

This paper formulates a field theory in the tradition of Gibbs (1878) and Biot (1941, 1973). We phrase the theory in terms of nonequilibrium thermodynamics (e.g., Prigogine, 1967; Coleman and Noll, 1963)

@article{doi:10.1098/rspa.2019.0761,

author = {Liu, Zezhou and Bouklas, Nikolaos and Hui, Chung-Yuen },

title = {Coupled flow and deformation fields due to a line load on a poroelastic half space: effect of surface stress and surface bending},

journal = {Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences},

volume = {476},

number = {2233},

pages = {20190761},

year = {2020},

doi = {10.1098/rspa.2019.0761},

URL = {https://royalsocietypublishing.org/doi/abs/10.1098/rspa.2019.0761},

eprint = {https://royalsocietypublishing.org/doi/pdf/10.1098/rspa.2019.0761}

}

@Article{Kang2010,

author ={Kang, Min K. and Huang, Rui},

title = {Effect of surface tension on swell-induced surface instability of substrate-confined hydrogel layers},

journal = {Soft Matter},

year = {2010},

volume ={6},

issue ={22},

pages = {5736-5742},

publisher = {The Royal Society of Chemistry},

doi ={10.1039/C0SM00335B},

url ={http://dx.doi.org/10.1039/C0SM00335B},

}

Here we present a theoretical model that predicts the critical condition along with a characteristic wavelength for swell- induced surface instability in substrate-confined hydrogel layers.

Swell-induced surface instability has been observed experimentally in rubbers and gels. Here we present a theoretical model that predicts the critical condition along with a characteristic wavelength for swell- induced surface instability in substrate-confined hydrogel layers.

Such instability may pose a fundamental limit on load-carrying capacity of rubber or on the degree of swelling for gels. On the other hand, the physics of surface instability may be harnessed in the design of responsive ‘‘smart’’ surfaces for novel applications.

The present study focuses on the effects of surface tension on both the critical condition and the characteristic wavelength.

@Article{Caldorera-Moore2011,

author = {Caldorera-Moore, Mary and Kang, Min Kyoo and Moore, Zachary and Singh, Vikramjit and Sreenivasan, S. V. and Shi, Li and Huang, Rui and Roy, Krishnendu},

title = {Swelling behavior of nanoscale{,} shape- and size-specific{,} hydrogel particles fabricated using imprint lithography},

journal = {Soft Matter},

year = {2011},

volume = {7},

issue = {6},

pages = {2879-2887},

publisher = {The Royal Society of Chemistry},

doi = {10.1039/C0SM01185A},

url = {http://dx.doi.org/10.1039/C0SM01185A},

}

One critical question on such approaches is whether in vivo swelling of the nanoparticles could considerably alter their geometry to a point where the potential benefit of controlling size or shape could not be realized.

Our results indicate a size-dependent swelling which can be attributed to the effect of substrate constraint of as-fabricated particles, when the particles are still attached to the imprinting substrate. Numerical simulations based on a recently developed field theory and a nonlinear finite element method were conducted to illustrate the constraint effect on swelling and drying behavior of substrate-supported hydrogel particles of specific geometries, and compared closely with experimental measurements. Further, we present a theoretical model that predicts the size-dependent swelling behavior for unconstrained sub-micron hydrogel particles due to the effect of surface tension.

The as-fabricated particles are taken as the relaxed state in a parallelepiped shape with the bottom surface fully constrained by the rigid substrate

@article{GurtinMurdoch1978,

title = {Surface stress in solids},

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volume = {14},

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@article{Javili2009,

title = "A finite element framework for continua with boundary energies. Part I: The two-dimensional case",

journal = "Computer Methods in Applied Mechanics and Engineering",

volume = "198",

number = "27",

pages = "2198 - 2208",

year = "2009",

issn = "0045-7825",

doi = "https://doi.org/10.1016/j.cma.2009.02.008",

url = "http://www.sciencedirect.com/science/article/pii/S0045782509000802",

author = "A. Javili and P. Steinmann",

keywords = "Boundary potentials, Surface tension",

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@article{doi:10.1142/S1758825115300011,

author = {Liu, Zishun and Toh, William and Ng, Teng Yong},

title = {Advances in Mechanics of Soft Materials: A Review of Large Deformation Behavior of Hydrogels},

journal = {International Journal of Applied Mechanics},

volume = {07},

number = {05},

pages = {1530001},

year = {2015},

doi = {10.1142/S1758825115300011},

URL = {https://doi.org/10.1142/S1758825115300011}

}

Being biocompatible, many applications have been developed for hydrogels in the past few decades. Early uses of hydrogels tap on its superior bio-compatibility over plastic materials [Wichterle and Lim, 1960]. Some examples include contact lenses, wound dressings and implants [Corkhill et al., 1989; Kuroyanagi, 1999; Wichterle and Lim, 1960].

With different monomers or constituent particles, hydrogels are able to undergo large deformation with a small change in environmental stimulus, but not limited to temperature, pH value, light, electric field, ionic strength and magnetic field [Aguilaret al., 2007; Jeong and Gutowska, 2002; Li and Kong, 2007; Meng and Hu, 2010]. These environmentally sensitive gels are also known as “smart hydrogels” and are more attractive than the traditional hydrogels, whose main attraction is its superabsorbency.

Gong’ group from Hokkaido University have successfully developed the highly strong, tough, and viscous hydrogels which have a hierarchically-ordered complex structure. These types of hydrogels will provide revolutionary applications over traditional hydrogels [Gong, 2010; Gong et al., 2003; Sun et al., 2013]. Their recent inventions of tough hydrogels demonstrated the potential as structural materials. These physical hydrogels have a combination of mechanical properties including stiffness, strength, toughness, fatigue resistance and self-healing, along with biocompatibility. Most recently, the Suo group from Harvard University has developed a new method for the synthesis of hydrogels from polymers forming ionically and covalently crosslinked networks [Keplinger et al., 2013].

@Article{Ahn2008,

author ="Ahn, Suk-kyun and Kasi, Rajeswari M. and Kim, Seong-Cheol and Sharma, Nitin and Zhou, Yuxiang",

title ="Stimuli-responsive polymer gels",

journal = {Soft Matter},

year = {2008},

volume = {4},

issue = {6},

pages = {1151-1157},

publisher = {The Royal Society of Chemistry},

doi = {10.1039/B714376A},

url = {http://dx.doi.org/10.1039/B714376A}

}

Polymer gels comprising either physical or chemical cross-links can undergo controlled and reversible shape changes in response to an applied field. The stimulus or external field applied may include thermal, electrical, magnetic, pH, UV/visible light, ionic or metallic interactions or combinations thereof.

@article{Javili2010,

title = {A finite element framework for continua with boundary energies. Part II: The three-dimensional case},

journal = {Computer Methods in Applied Mechanics and Engineering},

volume = {199},

number = {9},

pages = {755 - 765},

year = {2010},

issn = {0045-7825},

doi = {https://doi.org/10.1016/j.cma.2009.11.003},

url = {http://www.sciencedirect.com/science/article/pii/S0045782509003788},

author = {A. Javili and P. Steinmann},

keywords = {Boundary potentials, Surface tension},

}

This paper, in line with part I [53], is concerned with the finite element implementation of boundary potential energies and the study of their impact on the deformations of solids thereby the main thrust is the fully three-dimensional formulation and implementation incorporating anisotropic effects.

Within this contribution the boundary potentials are allowed, in general, to depend not only on the boundary deformation but also on the boundary deformation gradient and the spatial boundary normal.

In this respect different behaviors for the surface of the continuum body can be considered by defining the respective surface potential energy which provides the possibility to model a wide variety of the materials, including fluids. Therefore, this methodology is sim- ilar to the latter approach introduced above. Next, the surface of the body resembles a membrane coupled with the bulk and possessing the surface elastic properties of Gurtin and Murdoch [5] which follows the methodology of the first approach.

@article{Kang2010FE,

author = {Kang, Min Kyoo and Huang, Rui},

title = "{A Variational Approach and Finite Element Implementation for Swelling of Polymeric Hydrogels Under Geometric Constraints}",

journal = {Journal of Applied Mechanics},

volume = {77},

number = {6},

year = {2010},

month = {08},

issn = {0021-8936},

doi = {10.1115/1.4001715},

url = {https://doi.org/10.1115/1.4001715}

}

In particular, the effect of geometric constraint is emphasized for the inhomogeneous swelling of surface-attached hydrogel lines of rectangular cross sections, which depends on the width-to-height aspect ratio of the line.

In Sec. 4, we first consider three simple examples of homogeneous swelling of a hydrogel; one, without constraint and, two, with constraint. Numerical results are compared with the corresponding analytical solutions as benchmarks for the finite element implementation. Next, inhomogeneous swelling of surface-attached hydrogel lines is considered to further emphasize the effect of geometric constraint.

@article{Roman2018Review,

author = {Bico, José and Reyssat, Étienne and Roman, Benoît},

title = {Elastocapillarity: When Surface Tension Deforms Elastic Solids},

journal = {Annual Review of Fluid Mechanics},

volume = {50},

number = {1},

pages = {629-659},

year = {2018},

doi = {10.1146/annurev-fluid-122316-050130},

URL = {https://doi.org/10.1146/annurev-fluid-122316-050130},

eprint = {https://doi.org/10.1146/annurev-fluid-122316-050130}

}

This review aims to describe the different scaling parameters and characteristic lengths involved in elastocapillarity. We focus on three main configurations, each characterized by a specific dimension: three-dimensional (3D), deformations induced in bulk solids; 1D, bending and bundling of rod-like structures; and 2D, bending and stretching of thin sheets.

Although negligible at large scales, capillary forces may become dominant for submillimetric objects.

However, beyond liquid interfaces, capillary forces can also deform solid bodies in their bulk, as observed in recent experiments with very soft gels.

At small scales (more precisely, at small Reynolds numbers), interactions between viscous forces and soft structures are important in the locomotion of microorganisms and can induce deformations of cells or blood vessels, as recently reviewed by Duprat & Stone (2015).

Recent technological advances in microfabrication and the development of very soft materials have motivated numerous studies of the coupling between surface tension and elasticity.

Many reviews have been dedicated to the self-assembly of small objects by capillary forces (Boncheva & Whitesides 2005, Mastrangeli et al. 2009) and to the collapse (Maboudian 1997) or folding (Syms et al. 2003, Leong et al. 2010, Crane et al. 2013) of engineered microstructures

Consequently, surface stresses in solids are, in principle, strain dependent.

Capillary-induced deformations also constitute a useful tool to probe the mechanics of biological cells, as recently reported by Campa`s et al. (2013).

For instance, the possible collapse of microstructures is an important constraint in the design of microelectromechanical systems (MEMS).

Although complex 2D structures are commonly obtained through conventional lithography, build- ing 3D micro-objects remains challenging. Capillary forces constitute a promising tool to self-assemble micro-objects in two and even in three dimensions (Boncheva & Whitesides 2005, Mastrangeli et al. 2009).

For instance, 3D photovoltaic cells obtained by capillary origami could exhibit enhanced yield (Guo et al. 2009), and self-folding microcontainers could be used to encapsulate drugs (Fernandes & Gracias 2012).

Biophysics—a field driven by better mechanical control at the cellular level—is particularly ripe for numerous upcoming applications. For instance, Campa`s et al. (2013) nicely demonstrate how capillary pressure may be used for in vivo probing of living cells. Tubes of biological membranes are also known to undergo an instability reminiscent of the elastocapillary instability of soft gels, which leads to the fragmentation of mitochondria through pearling (Gonzalez-Rodriguez et al. 2015). The development of micro- and nanoengineered mechanical devices is also likely to raise new elastocapillary problems.

author = {Style, Robert W. and Jagota, Anand and Hui, Chung-Yuen and Dufresne, Eric R.},

title = {Elastocapillarity: Surface Tension and the Mechanics of Soft Solids},

journal = {{A}nnual {R}eview of {C}ondensed {M}atter {P}hysics},

volume = {8},

number = {1},

pages = {99-118},

year = {2017},

doi = {10.1146/annurev-conmatphys-031016-025326},

URL = {https://doi.org/10.1146/annurev-conmatphys-031016-025326},

eprint = {https://doi.org/10.1146/annurev-conmatphys-031016-025326}

}

It is widely appreciated that surface tension can dominate the behavior of liquids at small scales. Solids also have surface stresses of a similar magnitude, but they are usually overlooked. However, recent work has shown that these can play a central role in the mechanics of soft solids such as gels.

Furthermore, exciting new applications are developing in surgery, tissue engineering, flexible electronics, and soft robotics (e.g., 1–8), often utilizing the fact that soft solids can exhibit mechanical phenomena that differ qualitatively from hard engineering materials (9). One key difference is that surface stresses, which play a minor role in the mechanics of stiff materials, can dominate the behavior of soft solids.

We restrict our attention to polymer gels and elastomers, which have been the focus of experimental studies of elastocapillary phenomena. Gels consist of cross-linked networks of polymer swollen by a solvent, whereas elastomers have no solvent.

The research reviewed in this manuscript has established that interfaces in soft solids carry sufficient surface stress to strongly influence and sometimes dominate mechanical phenomena. Collectively, we use the term elastocapillarity to represent these phenomena.

For example, the Eshelby theory (which we have seen is strongly modified by surface stress) is widely used beyond composite mechanics, for example, in plasticity (127), fracture mechanics (128) and cell mechanics (129, 130), so surface stress may play a role in these phenomena. In particular, theory suggests that surface stress can strongly attenuate the energy release to a crack tip and thus effectively increase resistance to fracture, but this remains to be tested experimentally. Many soft materials exhibit plasticity, so we expect a whole range of plastocapillary effects, but this area is in its infancy (131, 132). Similarly, much biological material is soft, so there is almost certainly a range of biophysical elastocapillary phenomena to be uncovered (e.g., 133).

@Article{Andreotti2016,

author ={Andreotti, Bruno and Bäumchen, Oliver and Boulogne, François and Daniels, Karen E. and Dufresne, Eric R. and Perrin, Hugo and Salez, Thomas and Snoeijer, Jacco H. and Style, Robert W.},

title ="Solid capillarity: when and how does surface tension deform soft solids?",

journal ={Soft Matter},

year ={2016},

volume ={12},

issue ={12},

pages ={2993-2996},

publisher ={The Royal Society of Chemistry},

doi ={10.1039/C5SM03140K},

url ={http://dx.doi.org/10.1039/C5SM03140K}

}

While the physical origins of the surface properties of many stiff solids are well understood, a systematic investigation of the surface properties of soft solids must be undertaken. We need to both quantify continuum-scale surface properties and reveal their molecular-scale origins.

However, a second contribution arises when the surface energy is strain-dependent, leading to the so-called Shuttleworth effect. In this case, the surface stress U not only depends upon the surface energy, g, but also its derivatives with strain, as U = g + dg/de.

Polymeric materials have been the dominant choice for experiments in the mechanics of soft solids. These materials feature a system-spanning cross-linked polymer network; this network may be swollen either by un-crosslinked polymer, or by a chemically-distinct solvent.

@Article{Henann2014,

author ={Henann, David L. and Bertoldi, Katia},

title ={Modeling of elasto-capillary phenomena},

journal = {Soft Matter},

year = {2014},

volume = {10},

issue = {5},

pages = {709-717},

publisher = {The Royal Society of Chemistry},

doi = {10.1039/C3SM52583J},

url = {http://dx.doi.org/10.1039/C3SM52583J}

}

Surface energy is an important factor in the deformation of fluids but is typically a minimal or negligible effect in solids. However, when a solid is soft and its characteristic dimension is small, forces due to surface energy can become important and induce significant elastic deformation. The interplay between surface energy and elasticity can lead to interesting elasto-capillary phenomena.

Typically for solids, volumetric elastic strain energy dominates, but in certain cases, the surface and elastic energy scales are comparable, leading to an interesting interplay.

Modeling of elasto-capillary phenomena requires (i) mathematically describing both the behavior of the surface and the bulk and (ii) numerical methods for solving the resulting system of equations in arbitrary settings.

stress and this has recently been demonstrated experimentally.

@article{Fernandes2012,

title = {Self-folding polymeric containers for encapsulation and delivery of drugs},

author = "Rohan Fernandes and David H. Gracias",

journal = {Advanced Drug Delivery Reviews},

volume = {64},

number = {14},

pages = {1579 – 1589},

year = {2012},

issn = {0169-409X},

doi = {https://doi.org/10.1016/j.addr.2012.02.012},

url = {http://www.sciencedirect.com/science/article/pii/S0169409X12000919}

}

Self-folding methods are important for drug delivery applications since they provide a means to realize 3D, biocompatible, all-polymeric containers with well- tailored composition, size, shape, wall thickness, porosity, surface patterns and chemistry.

In drug delivery it is often required to package therapeutic cargo including small molecules, peptides, proteins, nucleic acids and living cells. Packaging provides a means to achieve enhanced solubility and accurate targeting, prevent premature degradation, permeate barriers, reduce dosage and limit side effects

The size and shape of the package strongly affect transport across different biological barriers and circulation times [26,27].

Many of these methods were initially developed in the microelectronics and microelectromechanical systems (MEMS) industries for use with metals, semiconductors and inorganic dielectrics, and are now being adapted for use with polymers and gels. Self-folding methods leverage the precision and versatility of existing planar micro and nanofabrication methods and additionally translate their capabilities into 3D, in a highly parallel manner.

A nonlinear, transient finite element method for coupled solvent diffusion and large deformation of hydrogels

Nikolaos Bouklas, Chad M. Landis, Rui Huang n

*Direct Quotes from introduction*

Hydrogels are capable of coupled mass transport and large deformation in response to external stimuli.

**2016**

**Dynamics of Swelling and Drying in a Spherical Gel**

Thibault Bertrand,1,\* Jorge Peixinho,2 Shomeek Mukhopadhyay,3 and Christopher W. MacMinn4,†

*Direct Quotes from introduction*

Swelling is a volumetric-growth process in which a porous material expands by spontaneous imbibition of additional pore fluid. Swelling is distinct from other growth processes in that it is inherently poromechanical: local expansion of the pore structure requires that additional fluid be drawn from elsewhere in the material, or into the material from across the boundaries.

A hydrogel is a cross-linked network of hydrophilic polymers saturated with water. Hydrogels can experience extremely large and reversible changes in volume during swelling, which can result in complex changes in shape and the development of surface patterns

In applications involving swelling, such as moisture absorption, drug delivery, and sensing and actuation, the primary design considerations are the degree of swelling and the rate of swelling in response to various environmental stimuli.

This is due in part to the fact that transient phenomena with large volume changes and strong poro- mechanical coupling are very challenging from the perspec- tive of computational mechanics.

Swelling reaches equilibrium when the penalty due to further stretching precisely balances the benefit due to further mixing.

**2015**

**Effect of Shape, Size, and Aspect Ratio on Nanoparticle Penetration and Distribution inside Solid Tissues Using 3D Spheroid Models**

*Rachit Agarwal,\* Patrick Jurney, Mansi Raythatha, Vikramjit Singh, Sidlgata. V. Sreenivasan, Li Shi, and Krishnendu Roy\**

*Direct Quotes from introduction*

**Efficient penetration and uniform distribution of nanoparticles (NPs) inside solid tissues and tumors is paramount to their therapeutic and diagnostic success.**

Nanoparticles are being investigated extensively for delivery of therapeutic and diagnostic agents. When encapsulated in, or conjugated to NPs, these agents could be protected from degradation and rapid clearance in the body and thus can be targeted to specific diseased cells and tissues with higher efficiency.

NPs allow for efficient intracel- lular delivery of the cargo, thereby pro- viding means to target specific cellular processes, signal transduction pathways, and organelle-specific molecules for both therapeutic and diagnostic applications.

Intravenous (IV) injection is the most common route for systemic delivery of NP-based drugs and imaging agents.

*Findings*

* Spherical NP penetration increases with decreasing size
* Low aspect ratio, cylindrical, disk-shaped particles are ideal for delivery and penetration into solid tissue

@Article{Caldorera-Moore2011,

author = {Caldorera-Moore, Mary and Kang, Min Kyoo and Moore, Zachary and Singh, Vikramjit and Sreenivasan, S. V. and Shi, Li and Huang, Rui and Roy, Krishnendu},

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}

One critical question on such approaches is whether in vivo swelling of the nanoparticles could considerably alter their geometry to a point where the potential benefit of controlling size or shape could not be realized.

Our results indicate a size-dependent swelling which can be attributed to the effect of substrate constraint of as-fabricated particles, when the particles are still attached to the imprinting substrate. Numerical simulations based on a recently developed field theory and a nonlinear finite element method were conducted to illustrate the constraint effect on swelling and drying behavior of substrate-supported hydrogel particles of specific geometries, and compared closely with experimental measurements. Further, we present a theoretical model that predicts the size-dependent swelling behavior for unconstrained sub-micron hydrogel particles due to the effect of surface tension.

The as-fabricated particles are taken as the relaxed state in a parallelepiped shape with the bottom surface fully constrained by the rigid substrate

The development of next-generation drugs, designed to interfere with specific cellular functions and pathways, has led to the demand for carriers that can efficiently and accurately deliver these agents to diseased cells or tissue while having minimal or no side effects.

To accommodate this need, a significant amount of research efforts have been put into the development of micro- and nanoparticles for protecting sensitive biological agents, targeting specific sites or biological conditions, and for envi- ronmentally triggered controlled release of encapsulated agents.

Hydrogels are cross-linked polymeric matrices that are widely utilized in a variety of biomedical applications primarily due to their high biocompatibility and their ability to be tailored for specific applications, including drug delivery.

Hydrogel materials are composed of hydrophilic polymeric networks that are crosslinked into a matrix like network either by chemical bonds or physical entanglements

Findings

* Bulk hydrogel properties are well known
* Characterizes in vivo selling of nanoscale hydrogel particles
* The results from the 100 nm particles support the hypothesis that there could be size-dependent swelling behavior when the nanoparticle dimensions are 100 nm or below; but further investigation of sub-100 nm hydrogel particles is needed to confirm this
* Theoretical analysis of the hydrogel swelling behavior results further demonstrate that the highly crosslinked PEGDA hydrogels do not swell significantly, and therefore the shape and size of these specific top-down fabricated nano-carriers can be preserved in aqueous environments (in vitro and in vivo settings) for particle size larger than 100 nm.

2010

REVIEW PAPER

**Chitosan-based hydrogels for controlled, localized drug delivery☆**

*Narayan Bhattarai 1, Jonathan Gunn 1, Miqin Zhang ⁎*

*Direct Quotes from introduction*

Despite the discovery of a large number of active compounds that could serve as therapeutics, very few candidates have shown clinical success. Poor activity in vivo is most often attributed to their low ‘bioavailability’, the extent and rate at which a drug reaches and affects target tissue.

Controlled delivery systems provide an alternative approach to regulating the bioavailability of therapeutic agents. In controlled drug delivery systems (DDSs), an active therapeutic is incorporated into a polymeric network structure in such a way that the drug is released from the material in a predefined manner

A variety of synthetic and natural polymers have been studied as drug carriers [5], and DDSs have capitalized on their wide-ranging hydrophobic and hydrophilic components, and their polymer–polymer, polymer–drug, polymer–solvent, or polymer–physiological medium interactions. While there are practically limitless combinations of materials to explore, engineers are restricted by material biocompatibility, toxic byproducts, surgical removal of DDSs, and manufacturing cost.

Hydrogels represent a DDS class that has excelled at intelligent drug delivery [5,6]. These gels are entangled polymer networks that trap a large amount of water without dissolving.

Fully swollen hydrogels have some physical properties common to living tissues, including a soft and rubbery consistency, and low interfacial tension with water or biological fluids. The elastic nature of fully swollen or hydrated hydrogels has been found to minimize irritation to the surrounding tissues after implantation. The low interfacial tension between the hydrogel surface and body fluid minimizes protein adsorption and cell adhesion, which reduces the chances of a negative immune reaction.

The swelling characteristics of a hydrogel is a key parameter in its use in diverse applications because the equilibrium swelling ratio (i.e. weight ratio of swollen hydrogel over the dry hydrogel) influences the solute diffusion coefficient, surface wettability and mobility, and the optical and mechanical properties of the hydrogel

Polymer binding is accomplished either by non-covalent physical associations, such as secondary forces (hydrogen, ionic, or hydrophobic bonding) and physical entanglements, or by covalent cross-linkages [5,25].

The physical properties of swollen hydrogels are regulated by the molecular weight (MW) of the polymer, charges on the polymers, density of the cross-linking (covalently bonded networks), and physical associations.

Findings

* Chitosen is a biocompatible polymer (very useful)
* Very chemistry focused paper