SWEDISH DEFENCE
RESEARCH AGENCY

FOI-R–1298–SE
August 2004
ISSN 1650-1942

Methodology report

Mattias Unosson and Lars Olovsson

Multiscale modelling of solid material mechanical behaviour

Weapons and protection division
SE-147 25 TUMBA

FOI – Swedish Defence Research Agency
Weapons and protection division
SE-147 25 TUMBA

FOI-R–1298–SE
August 2004
ISSN 1650-1942

Methodology report

Mattias Unosson and Lars Olovsson

Multiscale modelling of solid material mechanical behaviour

Weapons and protection division
SE-147 25 TUMBA

Abstract

A brief review is given on existing theories for modelling matter on different length scales. A process and a terminology for the modelling is proposed to be used in all the scientific and engineering disciplines. The methods for multiscale modelling developed need to be improved as well as computer performance has to grow before it can be used in product development. However, multiscale modelling can lend new insights to engineer new materials with optimal properties for any application.

Contents

1 Introduction

Modelling of material at different length scales can become a powerful tool in the development of new materials with optimal and engineered properties. Analysis on different length scales may also be used to explain macroscopic mechanical behaviour in terms of structure on atomic or molecular level.

A process and a terminology for modelling solid material mechanical behaviour is presented here to serve as a connector between researchers from different scientific and engineering disciplines. The experience of the authors is that the lack of a common language, apart from mathematics, makes it difficult for different research groups to interact.

Scientific theories and hypotheses are often in the form of models and are commonly divided into analogue, iconical and symbolical models. Analogue models lack structural resemblance with the parent object, while iconical models are scaled projections of the same. Symbolical models are almost exclusively mathematical and it is also the type of model scrutinized here. It would be impossible to capture the true nature of matter in a model since our perception of the world is limited by our senses and by instrument technology. But, even a model incorporating only intersubjective scientific knowledge on matter received through these senses and instruments would be too large for practical use. In *Gulliver's travels* Swift portrays how the map makers, in their strive not to miss any details, constructs a map of their country as large as the country itself. Even though their model is iconical and not mathematical, the story points out the necessity to introduce some degree of idealization and the first is a restriction to the world as described by physics.

2 Philosophy of modelling

The proposed process for the mathematical modelling of material, from the real world to the validation of computational results against experimental results, is divided into five sub-processes, see Figure 1.

2.1 Idealization

Idealizations are here made in four dimensions; conceptual, mathematical treatment, spatial and temporal.

Conceptual

In physics there are four closed sets of concepts, cf. Figure 2. Thermodynamics can easily be connected to any of the other sets and classical mechanics is related to two of the others as limiting cases. In the first case velocities are infinitely low in comparison with the speed of light and in the second case Planck's constant can be considered as infinitely small. The theory of general relativity is still an open mathematical set and only relevant when strong acceleration fields are present. See Heisenberg [1] for a detailed discussion on these concepts and their relations.

Errors generated by classical mechanics compared to the special theory of relativity are of order $(v/c)^2$, where v is the current velocity and c the speed of light, cf. Synge [2]. Only if relativistic effects can be ignored is it possible to uncouple time and space and treat them separately in the classic manner. The error, or rather uncertainty, generated by classical mechanics compared to quantum mechanics is governed by the Heisenberg's relation

$$\Delta p_i \Delta x_i \geq \frac{1}{2}\hbar \tag{1}$$

where Δp_i and Δx_i are the uncertainties in momentum and position respectively and $\hbar$ is Planck's constant divided by 2π. This relation restricts the time of observation of classical mechanics at smaller spatial scales.

Mathematical treatment

Further, in physics there are two viewpoints in the mathematical treatment of matter; discrete theories and field theories. Discrete theories describe matter as discontinuous while in field theories matter is represented by continuous functions. If discontinuities are present in a field theoretical model jump conditions are introduced, cf. Truesdell and Toupin [3].

Some concepts belongs inherently to one or the other viewpoint, for example is thermodynamics a field theory and quantum mechanics is a combination of both field and discrete elements. With classical mechanics the choice lie open.

Spatial

The model is spatially limited to encompasss only a part of the world and matter outside this finite, spatial control domain influences the phenomenon only through imposed boundary conditions and gravitational fields.

An inner spatial, or material, scale also has to be chosen, see Figure 3. The internal spatial scales are different for metallic, ceramic, polymeric and composite materials but, in Figure 3 metallic materials are used as reference.

Some theories belongs inherently to a spatial scale, for example are classical thermodynamics, optics and magnetism macroscopic scale theories.

Temporal

If the process studied is dynamic the past is reduced to initial conditions and the phenomenon is studied over a finite, temporal control domain. As mentioned before, use of classical mechanics limits the size of the temporal domain.

2.2 Discretization

If a sufficiently high degree of idealization is made then, the model will be analytically solvable. But, to solve more complex models numerical analysis on computers has to be used where the idea is to efficiently calculate accurate approximations to the solution. However, computers work with finite sets and discretization of the infinite sets in the model into finite sets constitutes therefor a basic element of numerical analysis. Discretization is performed of either the temporal control domain or the spatial control domain or both. If integrational expressions have to be evaluated then, numerical integration has to be used. All this induces indirectly idealizations of the real world.

2.3 Implementation

Computers do work linearly but, model input consists frequently of nonlinear functions. Algorithms have to be used that perform iterations on linear, finite sets to implement the model. This also induces indirect idealizations of the real problem.

2.4 Simulation

The accuracy of the result from the simulation depends to some extent on the precision of the computer used. A simulation consists of three activities; preprocessing to generate code input, execution of the implemented code and postprocessing to visualize the results.

2.5 Validation

The computational result is visualized and compiled in order to perform a validation against experimental observations. When experimental data is prepared for comparison it must often be filtered, which can introduce errors.

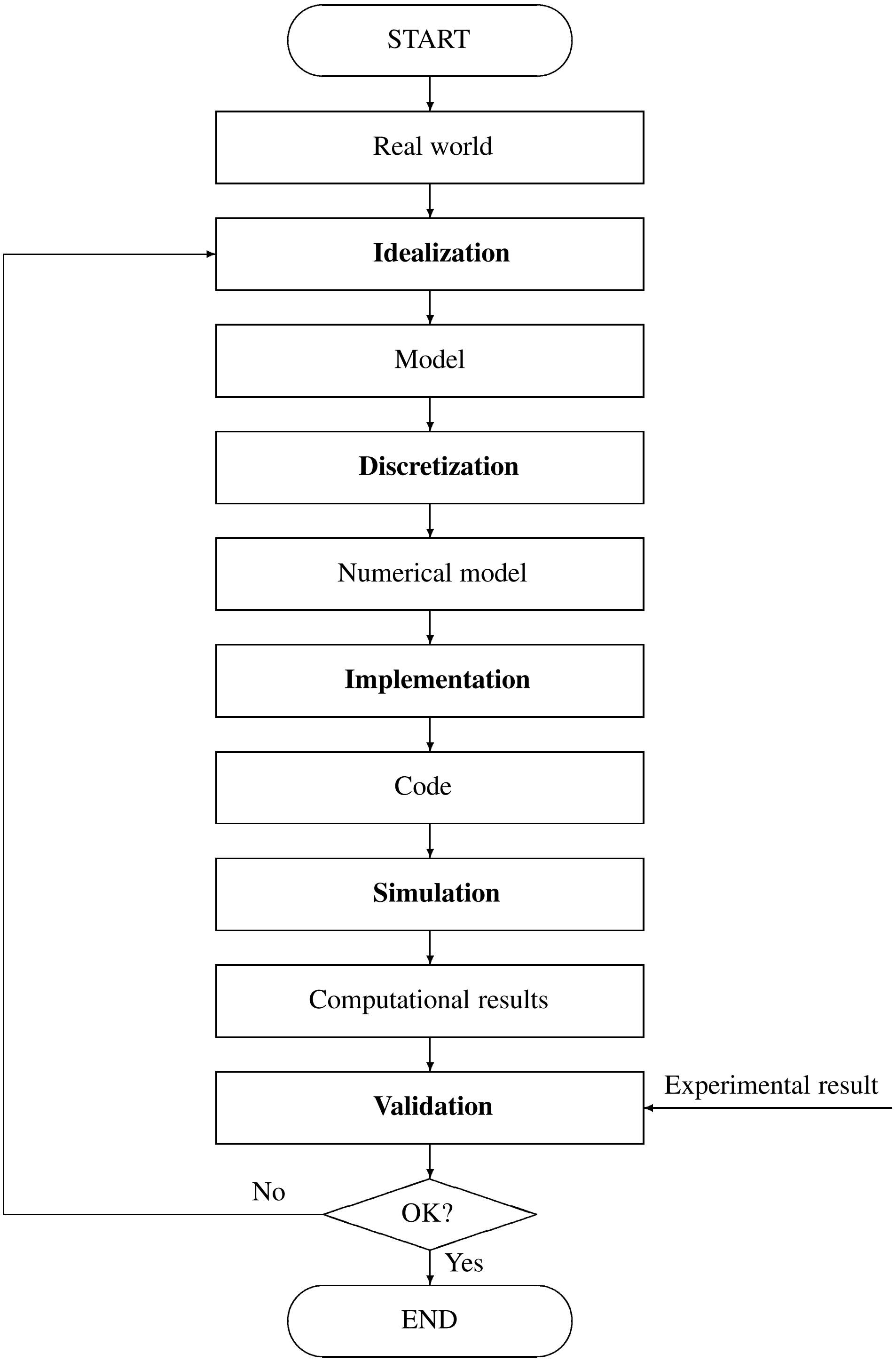

Figure 1. Process of modelling

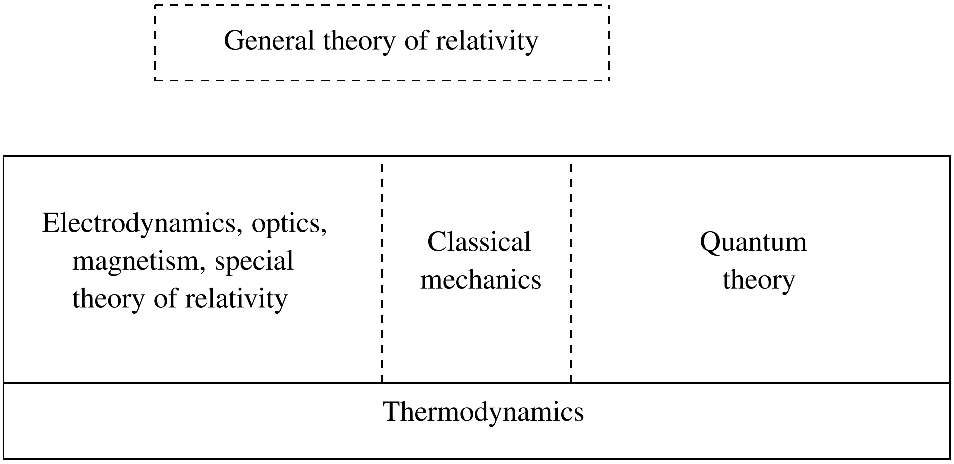

Figure 2. Concepts of physics

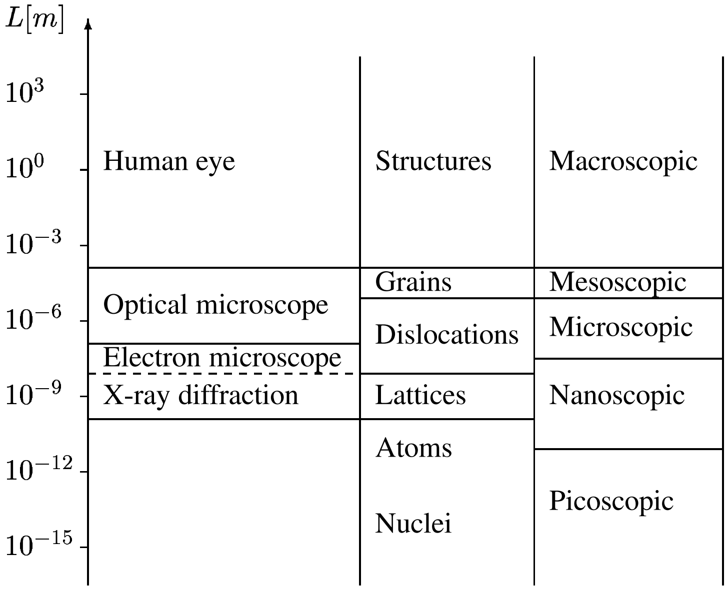

Figure 3. Material scales for metallic materials

3 Multiscale modelling

A process for multiscale modelling is shown in Figure 4 and for every sub-process a brief overview is given below. Also, see Figure 3 for material scale references.

3.1 Pico - Quantum mechanics

(Concept: Quantum theory, Treatment: Field- and discrete theory, Spatial: Picoscopic, Temporal: Limited by relativity)

The cohesion or binding energy of solids is entirely due to the attractive electrostatic interaction between the negative charges of the electrons and the positive charges of the nuclei. Given the spatial distribution and the velocity distribution of electrons and nuclei in their free state and in a crystal respectively, it is possible to calculate the binding energy in a crystal, cf. Kittel [4]. Non-relativistic quantum mechanics is mainly concerned with solving the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\mathbf{x},t) + V(\mathbf{x},t)\Psi(\mathbf{x},t) = i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t) \tag{2}$$

where m is the particle mass, $V(\mathbf{x},t)$ is the potential field in which the particle is moving, $\Psi(\mathbf{x},t)$ is the particle wave function and

$$|\Psi(\mathbf{x},t)|^2 \tag{3}$$

is the particle probability distribution. One can assume that the wave function is separable, such that it can be expressed as the product of one spatial function and one time function.

$$\Psi(\mathbf{x},t) = \psi(\mathbf{x})\tau(t) \tag{4}$$

Further, assuming V is not a function of time and τ is the harmonic function

$$\tau(t) = \mathrm{e}^{-i\omega t} \tag{5}$$

equations (2) and (5) lead to the time-independent Schrödinger equation.

$$H\psi(\mathbf{x}) = E\psi(\mathbf{x}) \tag{6}$$

where

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) \tag{7}$$

is the Hamiltonian operator and

$$E = \hbar\omega \tag{8}$$

is the energy of the particle. Considering a configuration of several atoms a number of approximations has to be made to solve Equation (6) and to compute the binding energy. From this it is possible to compute macroscopic elastic material properties, cf. for example Vitos et al. [5] for steel alloys.

3.1.1 Approximations

It is generally assumed that the nuclei is static and that its mass is infinitly larger than the mass of the surrounding electrons. Still, finding an accurate numerical solution to the Scrödinger equation for many electrons interacting with each other is not a trivial task. However, the total number of equations to solve can be greatly reduced by, as in the pseudo-potential (PP) method, assuming that only the valence electrons need to be considered.

Further, the density functional theory (DFT) simplifies the numerical solution to a multi-electron Schrödinger equation. The theory is based on simplifying the influence from the surrounding on an electron through the definition of an effective nuclei potential $V(\mathbf{x})$ [6]. However, a good effective nuclei potential is generally not trivially defined.

With the local density approximation (LDA), the effective nuclei potential is defined as a function of the local electron density [7]. In an extension to the LDA approximation, the generalized gradient approximation (GGA) [8], the effective nuclei potential is defined as a function of both the local electron density and of its gradient.

3.2 Nano - Molecular dynamics

(Concept: Classical mechanics, Treatment: Field- and discrete theory, Spatial: Nanoscopic, Temporal: Limited by uncertainty and relativity)

Molecular dynamics (MD) is based on classical Newtonian mechanics where each atom is modeled as a concentrated mass m at a distinct coordinate in space. The acceleration $\mathbf{a}$ of an atom is defined as

$$\mathbf{a} = \frac{\mathbf{F}}{m} \tag{9}$$

where $\mathbf{F}$ is the total force acting on the atom. $\mathbf{F}$ is an interaction force that is derived from gradients of inter-atomic energy potentials. The potentials are generally fitted to quantum mechanical simulation results and to known material data.

3.2.1 Energy potentials

In the embedded atom method (EAM) the energy potentials are defined as functions of the pairwise distance between the atoms and of a background electron density [9].

$$E_{tot} = \sum_i F(\rho_i) + \frac{1}{2}\sum_{ij}{}' \phi_{ij}(r_{ij}) \tag{10}$$

$(i, j) \in [1, N] \times [1, N]$, where N is the total number of atoms considered. E_{tot} is the total atom bonding energy of the system and ϕ_{ij} is a pairwise energy potential that is a function of the distance r_{ij} between atoms i and j. The prime on the second sum excludes all self-interaction terms where two indices are equal. F is a universal function that does not depend on the source of the background electron density ρ_i, [9].

$$\rho_i = \sum_{j \neq i} \bar{\rho}_j(r_{ij}) \tag{11}$$

where $\bar{\rho}_j$ is the background electron density contribution from atom j.

EAM assumes only radial interaction forces between the atoms. The advantage of the formulation is relatively simple potential functions, from which the pairwise acting atom forces easily can be derived. According to literature [10] EAM works well for realtively noble transition metals. That is, metals with filled, or nearly filled, d-shells.

For other metals, where a directional bonding is more pronounced, more complex potential functions are necessary. In this context, it is worth mentioning the generalized pseudopotential method (GPT) and the model generalized pseudopotential method (MGPT) [10]. For a pure metal the GPT defines the energy as

$$\begin{aligned} E_{tot} = NE_{vol}(\Omega) + \frac{1}{2}{\sum_{ij}}' v_2(ij;\Omega) + \frac{1}{6}{\sum_{ijk}}' v_3(ijk;\Omega) + \\ \frac{1}{24}{\sum_{ijkl}}' v_4(ijkl;\Omega) + ... \end{aligned} \tag{12}$$

where

$$\begin{aligned} v_2(ij;\Omega) &= v_2(r_{ij},\Omega) \\ v_3(ijk,\Omega) &= v_3(r_{ij},r_{jk},r_{ki},\Omega) \\ v_4(ijkl;\Omega) &= v_4(r_{ij},r_{ik},r_{il},r_{jk},r_{jl},r_{kl},\Omega) \end{aligned} \tag{13}$$

N and Ω are the number of atoms and the atomic volume, respectively.

With todays computer resources, only very small material volumes can be modelled. Due to the size of dislocation structures in crystalline metal alloys, molecular dynamics can hardly be used to simulate large plastic deformations of this class of materials. The modelling technique is better suited for amorphous metals, where the mechanisms governing plastic flow are completely different.

3.3 Micro - Dislocation dynamics

(Concept: Classical mechanics, Treatment: Field- and discrete theory, Spatial: Microscopic, Temporal: Limited by relativity but practically unlimited by uncertainty)

In dislocation dynamics the discrete treatment of single atoms is abandoned, c.f. Devrince et al. [11]. Instead, the core material is modelled as an elastic continuum, into which the dislocations are embedded as explicitly described one-dimensional structures. A dislocation dynamics model is completed by assumptions regarding the dislocation activation stresses and their interaction properties. This approach readily allows the study of micrometer sized structures. However, defining the dislocation properties is not a trivial task.

Inelastic defomations of amorphous materials are not related to the migration, growth and annihilation of dislocation structures. Consequently, dislocation dynamics is not a feasible way of modelling this class of materials.

3.4 Meso - Crystal plasticity

(Concept: Classical mechanics, Treatment: Field theory, Spatial: Mesoscopic, Temporal: Limited by relativity but practically unlimited by uncertainty)

In crystal plasticity, the material is viewed as a continuum where plastic deformations are imposed by the activation of crystallographic glide planes. Working on a mesoscopic scale, each grain in the crystal is modelled individually and the technique can be used to predict the development of crystallographic texture and grain geometries. Incorporating the migration of dislocations in the model, crystal plasticity also has the potential to bring insight into the relationship between grain size and macroscopic response of a specific alloy, cf. Olovsson [12].

However, crystal plasticity is of little or no use as a tool to predict or describe the material behavior on a microscopic level.

3.5 Macro - Continuum mechanics

(Concept: Classical mechanics, Treatment: Field theory, Spatial: Macroscopic, Temporal: Limited by relativity but practically unlimited by uncertainty)

Macro scale modelling is generally based on continuum mechanical assumptions and on material homogenity. Modelling on this level is of little or no use at all if one aims at predicting or explaining the properties of a specific material. It is merely used to explain or predict the response of mechanical structures at different initial and boundary conditions.

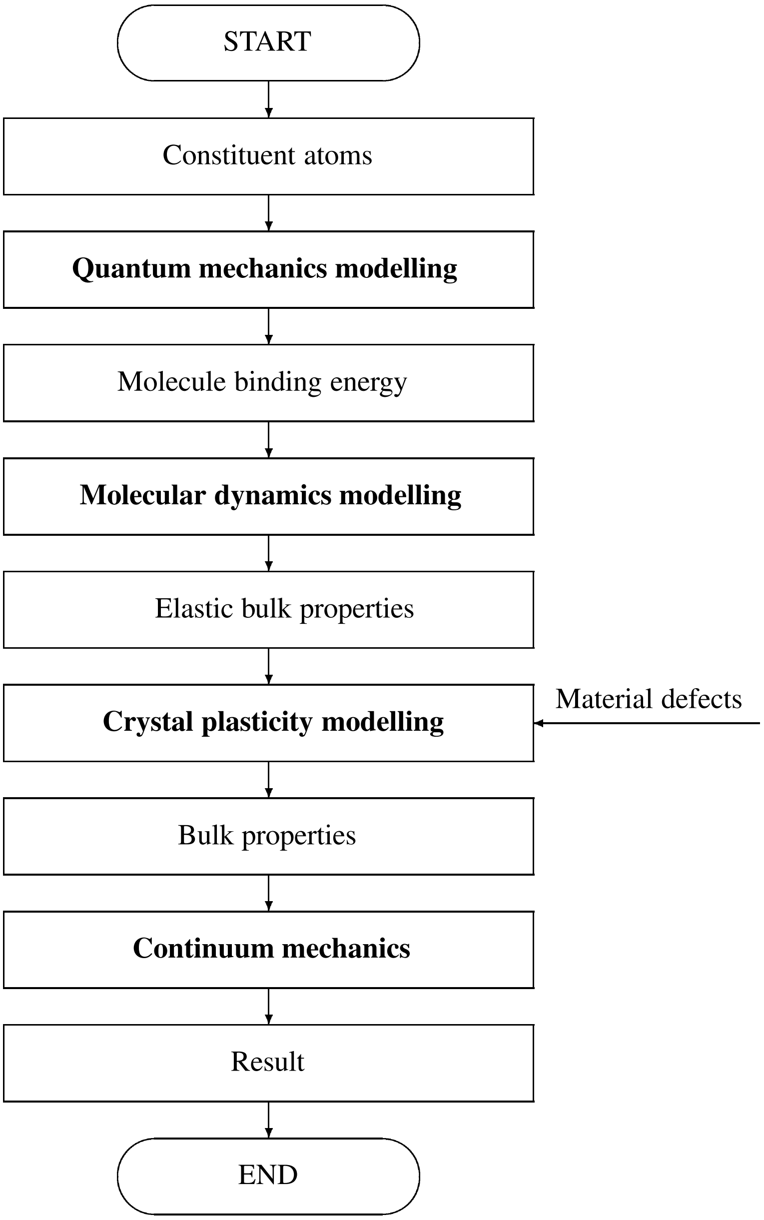

Figure 4. Scheme for multiscale modelling of metals

4 Discussion

Multiscale modelling is today mainly an activity within the research community, where it receives attention by physicists and engineers at a growing rate. The methods developed need however to be improved as well as computer performance has to grow before use of multiscale modelling in commercial product development will be a reality. But, already there are journals and conferences devoted to multiscale modelling

When these methods are mature and the computational capabilities suffice, they will together lend new and tremendous possibilities to understand and engineer new materials with optimal properties for any application. At this point we will most likely have a more profound integration of for example physics, solid mechanics and engineering material science that renders new insights into each others world of thinking.

References

[1] W. Heisenberg, *Physics and philosophy: The revolution in modern science*. Great minds series, Amherst, NY: Prometheus books, 1999. Original publication, Amherst, N.Y. : Harper & Row, 1958.

[2] J. L. Synge, "Classical dynamics," in *Encyclopedia of physics* (S. Flügge, ed.), vol. III/1, pp. 1–225, Berlin-Göttingen-Heidelberg: Springer-Verlag, 1960.

[3] C. A. Truesdell and R. A. Toupin, "The classical field theories," in *Encyclopedia of physics* (S. Flügge, ed.), vol. III/1, pp. 226–793, Berlin-Göttingen-Heidelberg: Springer-Verlag, 1960.

[4] C. Kittel, *Introduction to solid state physics*. New York: Wiley, third ed., 1966.

[5] L. Vitos, P. A. Korzhavyi, and B. Johansson, "Modeling of alloy steels," *Materials Today*, vol. 5, no. 10, pp. 14–23, 2002.

[6] H. Hohenberg and W. Kohn, "Inhomogeneous electron gas," *Physical review*, vol. 136, no. 3B, pp. B864–B871, 1964.

[7] W. Kohn and L. Sham, "Self-consistent equations including exchange and correlation effects," *Physical review*, vol. 140, no. 4A, pp. A1133–A1138, 1965.

[8] J. P. Perdew, J. Chevary, S. Vosko, K. A. Jackson, M. R. Pederson, D. Singh, and C. Fiolhais, "Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation," *Physical Review*, vol. B46, no. 11, pp. 6671–6687, 1992.

[9] H. Rafii-Tabar, "Modelling the nano-scale phenomena in condensed matter physics via computer-based numerical simulations," *Physics Reports*, vol. 325, no. 6, pp. 239–310, 2000.

[10] J. A. Moriarty, J. F. Belak, R. E. Rudd, P. Söderlind, F. H. Streitz, and L. H. Yang, "Quantum-based atomistic simulation of materials properties in transition metals," Preprint UCRL-JC-146608, Lawrence Livermore national laboratories, Jan. 8, 2002.

[11] B. Devincre, L. Kubin, C. Lemarchand, and R. Madec, "Mesoscopic simulations of plastic deformation," *Materials science and engineering A*, vol. 309-310, pp. 211–219, 2001.

[12] L. Olovsson, "KRYP, a finite element tool for crystal plasticity analyses," Methodology report FOI-R–0374–SE, Swedish defence research agency, Stockholm, Mar. 2002.

Issuing organisation FOI – Swedish Defence Research Agency Weapons and protection division SE-147 25 TUMBA	Report number, ISRN FOI-R–1298–SE	Report type Methodology report
	Month year August 2004	Project number I254
	Customers code 5. Commissioned research	
	Research area code 5. Combat	
	Sub area code 51. Weapons and Protection	
Author(s) Mattias Unosson and Lars Olovsson	Project manager Peter Skoglund	
	Approved by Michael Jacob Manager, Protection and material	
	Scientifically and technically responsible -	
Report title Multiscale modelling of solid material mechanical behaviour		

Abstract

A brief review is given on existing theories for modelling matter on different length scales. A process and a terminology for the modelling is proposed to be used in all the scientific and engineering disciplines. The methods for multiscale modelling developed need to be improved as well as computer performance has to grow before it can be used in product development. However, multiscale modelling can lend new insights to engineer new materials with optimal properties for any application.

Keywords
material modelling, multiscale modelling, solid matter, mechanical properties

Further bibliographic information

ISSN ISSN 1650-1942	Pages 25	Language English
	Price According to price list	
	Security classification Unclassified	

Utgivare Totalförsvarets Forskningsinstitut – FOI Avdelningen för vapen och skydd 147 25 TUMBA	Rapportnummer, ISRN FOI-R–1298–SE	Klassificering Metodrapport
	Månad år Augusti 2004	Projektnummer I254
	Verksamhetsgren 5. Uppdragsfinansierad verksamhet	
	Forskningsområde 5. Bekämpning	
	Delområde 51. VVS med styrda vapen	
Författare Mattias Unosson and Lars Olovsson	Projektledare Peter Skoglund	
	Godkänd av Michael Jacob Chef, Skydd och material	
	Tekniskt och/eller vetenskapligt ansvarig -	

Rapporttitel

Flerskalemodellering av fasta materials mekaniska beteende

Sammanfattning

En översikt över existerande teorier för modellering av materia ges, med inriktning mot fasta material och mekaniska egenskaper. En process och terminologi för modelleringen föreslås som skall kunna användas i alla vetenskaps- och teknikområden. De metoder för flervinåmodellering som utvecklas måste dock förbättras likväl som beräkningskapaciteten måste öka för att de skall kunna tillämpas i produktutveckling. Men, flernivåmodellering kan komma att ge ny insikter i hur man skräddarsyr material med optimala egenskaper för specifika tillämpningar.

Nyckelord

materialmodellering, flerskalemodellering, fast materia, mekaniska egenskaper

Övriga bibliografiska uppgifter

ISSN ISSN 1650-1942	Antal sidor 25	Språk Engelska
Distribution enligt missiv -	Pris Enligt prislista	
	Sekretess Öppen	